Science Supplementary Material
SM358 The Quantum World

SM358

Further Exercises

Contents

This collection of exercises is based on a bank of questions formerly used in problem classes at Open University Residential Schools. The problem classes were designed to support SM358. They concentrate mainly on the first half of SM358, and do not include many-particle systems, entanglement or most of the Book 3 topics, but they are all relevant for your studies. You can use them for further practice or revision, or you can treat them as worked examples.

Questions

A: Schrödinger's equation

Question A1

(a) Write down Schrödinger's equation for a free particle of mass m.

(b) Show that the function $\Psi(x,t) = A\exp(\mathrm{i}(kx-\omega t))$, where k and ω are constants, satisfies the equation you wrote down in part (a) provided that ω and k obey a relationship, which you should derive.

Question A2

A system with Hamiltonian operator

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

is in a state described by the wave function

$$\Psi(x,t) = \psi(x)\,T(t),$$

where $\psi(x)$ obeys the time-independent Schrödinger equation $\widehat{\mathrm{H}}\psi(x) = E\psi(x)$, with energy eigenvalue E. Use this information to derive an expression for the time-dependent factor $T(t)$ in the wave function.

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B: The time-independent Schrödinger equation

Question B1

(a) Write down the time-independent Schrödinger equation for a particle of mass m moving in a one-dimensional infinite square well with potential energy equal to zero in the region $-a \leq x \leq a$, and infinity otherwise. State the boundary conditions for this equation at $x = \pm a$.

(b) Show that the function

$$\psi(x) = \begin{cases} A\cos(5\pi x/2a) & \text{for } -a \leq x \leq a, \\ 0 & \text{otherwise} \end{cases}$$

satisfies this equation and its associated boundary conditions, and find the energy, E, of the corresponding state.

(c) Find a value of the normalization constant A.

(d) What is the probability of finding the particle in the interval $-0.2a \leq x \leq 0.2a$?

You may find the following integral useful:

$$\int_{-n\pi/2}^{n\pi/2} \cos^2 u \, \mathrm{d}u = \frac{n}{2}\pi \quad \text{for } n = 1, 2, 3, \ldots.$$

Question B2

(a) Write down the time-independent Schrödinger equation for a particle of mass m moving in a one-dimensional infinite square well with potential energy equal to zero in the region $0 \leq x \leq L$, and infinity otherwise.

(b) Show that the function

$$\psi(x) = A\sin[(2mE)^{1/2}x/\hbar] + B\cos[(2mE)^{1/2}x/\hbar] \quad (0 \leq x \leq L)$$

is a solution inside the well, where E is the total energy of the particle, and A and B are constants.

(c) Deduce as much information as you can from the boundary conditions.

(d) Find a value of the constant A which ensures that $\psi(x)$ is normalized.

(e) Suppose that the particle is in the second excited state. Write down the stationary-state wave function for this state as a function of position and time.

(f) Write down the probability density function for the second excited state, and determine the probability of finding the particle in the interval $0 \leq x \leq L/9$.

You may find the following indefinite integral useful:

$$\int \sin^2 u \, \mathrm{d}u = \tfrac{1}{2}u - \tfrac{1}{4}\sin(2u) + C,$$

where C is an arbitrary constant.

Question B3

(a) Write down the time-independent Schrödinger equation for a particle of mass m in a one-dimensional harmonic oscillator well with a force constant C.

(b) Show that the function $\psi(x) = x\exp[-x^2/2a^2]$, where $a^2 = \hbar/\sqrt{mC}$, is a solution of this time-independent Schrödinger equation. Show that the corresponding energy eigenvalue is $3\hbar\omega_0/2$, where $\omega_0 = (C/m)^{1/2}$.

(c) Normalize the function of part (b). Write down the corresponding normalized stationary-state wave function for any time t.

You may use the following integral:

$$\int_{-\infty}^{\infty} u^2 \exp(-u^2) \, \mathrm{d}u = \frac{\sqrt{\pi}}{2}.$$

Question B4

(a) Write down the time-independent Schrödinger equation for a particle of mass m in a well with potential energy function $V(x) = \frac{1}{2}Cx^2$.

(b) Show that the function $\psi(x) = A\exp(-x^2/2a^2)$, where $a^2 = \hbar/\sqrt{mC}$, is a solution of this time-independent Schrödinger equation. Calculate the energy E in terms of the classical angular frequency, $\omega_0 = \sqrt{C/m}$.

(c) Find a constant A (in terms of a) which normalizes $\psi(x)$.

(d) Is $\psi(x)$ an odd function, an even function, or neither?

(e) Show that, in this well, a classical particle of mass m, with the energy E calculated in part (b), in confined to the region $-a \leq x \leq a$.

(f) Find the quantum mechanical probability, correct to 3 significant figures, that the particle will be found within the classical limits.

You may use the integrals

$$\int_{-\infty}^{\infty} \exp(-u^2)\,\mathrm{d}u = \sqrt{\pi} \quad \text{and} \quad \int_0^1 \exp(-u^2)\,\mathrm{d}u = 0.747.$$

C: Eigenfunctions, expectation values and uncertainties

Question C1

A simple harmonic oscillator has a first excited state described by the energy eigenfunction

$$\psi(x) = N(2x/a)\exp(-x^2/2a^2),$$

where N is a normalization constant and a is the length parameter of the oscillator.

(a) Show that an appropriate value for N is $1/(2a\sqrt{\pi})^{1/2}$.

(b) Is $\psi(x)$ an odd function, an even function or neither? Show that the expectation values of x and p_x are both equal to zero in the state described by $\psi(x)$.

(c) Find the uncertainty in position, Δx in the state $\psi(x)$.

You may find the following integrals useful:

$$\int_{-\infty}^{\infty} u^2\exp(-u^2)\,\mathrm{d}u = \frac{\sqrt{\pi}}{2} \quad \text{and} \quad \int_{-\infty}^{\infty} u^4\exp(-u^2)\,\mathrm{d}u = \frac{3\sqrt{\pi}}{4}.$$

Question C2

(a) The energy eigenfunctions in a one-dimensional *symmetric* well are either even or odd functions. Use this fact to show that $\langle x\rangle = 0$ and $\langle p_x\rangle = 0$ for any stationary state of a one-dimensional *symmetric* well.

(b) Show that $\langle A\rangle$ is independent of time in any stationary state for any observable A.

(c) Show that the uncertainty in the energy of a stationary state is zero.

(d) Use the identity

$$\psi(x)\frac{\mathrm{d}\psi}{\mathrm{d}x} = \frac{1}{2}\frac{\mathrm{d}\psi^2}{\mathrm{d}x}$$

to show that $\langle p_x\rangle = 0$ for any real-valued bound-state wave function $\psi(x)$. You may use the fact that any bound-state wave function tends to zero at $\pm\infty$.

Question C3

(a) Show that $\psi_{k_x}(x) = (2\pi)^{-1/2}\exp(\mathrm{i}k_x x)$ is a solution of the eigenvalue equation

$$\widehat{\mathrm{p}}_x\psi_{k_x}(x) = p_x\psi_{k_x}(x),$$

where $\widehat{\mathrm{p}}_x$ is the momentum operator and p_x is a real number.

(b) Show that this solution is also an eigenfunction of the free-particle Hamiltonian, and that the degree of degeneracy is two.

(c) In a paragraph, explain why $\psi_{k_x}(x)$ cannot represent a free-particle state at any fixed time, and how the problem of the representation of free-particle states is resolved.

Question C4

A particle is confined in an infinite square well potential with walls at $-L/2$ and $L/2$. In the first excited state of this well, the normalized energy eigenfunction is

$$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) \quad \text{for } -L/2 \leq x \leq L/2,$$

and is equal to zero for $|x| > L/2$.

You may find the following integrals useful:

$$\int_{-\pi}^{\pi} u^2 \sin^2 u \, \mathrm{d}u = \frac{\pi^3}{3} - \frac{\pi}{2} \quad \text{and} \quad \int_{-\pi}^{\pi} \sin^2 u \, \mathrm{d}u = \pi.$$

(a) Determine the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$, and hence the uncertainty Δx in the state ψ_2.

(b) Determine the expectation values $\langle p_x \rangle$ and $\langle p_x^2 \rangle$, and hence the uncertainty Δp_x in the state ψ_2.

(c) Show that your answers to parts (a) and (b) are consistent with the uncertainty principle.

D: Wave packets

Question D1

The state of a harmonic oscillator is described by the wave function

$$\psi(x) = c_0\psi_0(x) + c_1\psi_1(x) + c_2\psi_2(x),$$

where $\psi_0(x)$, $\psi_1(x)$ and $\psi_2(x)$ are energy eigenfunctions with quantum numbers $n = 0$, $n = 1$ and $n = 2$, respectively. The corresponding energy eigenvalues are $E_n = (n + \frac{1}{2})\hbar\omega_0$, where ω_0 is the classical angular frequency. The constants c_0, c_1 and c_2 satisfy the normalization condition $|c_0|^2 + |c_1|^2 + |c_2|^2 = 1$.

You may use the fact that

$$\widehat{\mathrm{x}} = \frac{a}{\sqrt{2}} \left(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger\right),$$

where the constant a is the length parameter of the oscillator.

(a) Find $\langle x \rangle$ in the given state, expressing your answer in terms of the constants a, c_0, c_1 and c_2.

(b) Evaluate your answer in the special case $c_1 = 0$.

(c) Evaluate your answer in the special case $c_0 = 1/\sqrt{2}$, $c_1 = 1/\sqrt{2}$ and $c_2 = 0$.

(d) Evaluate your answer in the special case $c_0 = 1/\sqrt{2}$, $c_1 = \mathrm{i}/\sqrt{2}$ and $c_2 = 0$.

Question D2

In this question, ψ_1 and ψ_2 are orthonormal energy eigenfunctions.

(a) At time $t = 0$, a particle is in a state represented by a function of the form

$$\Psi(x, 0) = A\left(\tfrac{1}{2}\psi_1(x) + \psi_2(x)\right),$$

where A is a constant. Find the value of A, assuming it to be real and positive. What other values of A are possible? Do all these values correspond to the same state?

(b) At time $t = 0$, a particle is in a state represented by a function of the form

$$\Psi(x, 0) = \tfrac{1}{2}\psi_1(x) + \alpha\psi_2(x),$$

Find the value of α, assuming it to be real and positive. What other values of α are consistent with the given information? Do all these values correspond to the same state?

Question D3

The state of a particle at any time t is represented by the wave packet

$$\Psi(x,t) = \frac{1}{\sqrt{2}}(\psi_1(x)\exp[-\mathrm{i}E_1t/\hbar] + \psi_2(x)\exp[-\mathrm{i}E_2t/\hbar])$$

where $\psi_1(x)$ and $\psi_2(x)$ are *real* orthonormal energy eigenfunctions with eigenvalues E_1 and E_2 respectively ($E_1 \neq E_2$). Show that the probability density is an oscillating function of time with period $h/|E_2 - E_1|$.

Question D4

(a) Find a constant A that normalizes the wave packet

$$\Psi(x,0) = A[\psi_0(x) - 2\psi_1(x) + \mathrm{i}\psi_3(x)]$$

where the $\psi_n(x)$ are the normalized energy eigenfunctions of the harmonic oscillator with quantum numbers $n = 0$, $n = 1$ and $n = 3$, and with energy eigenvalues $E_n = (n + \frac{1}{2})\hbar\omega_0$, where ω_0 is the classical angular frequency of the oscillator.

(b) What is the probability of finding the value $3\hbar\omega_0/2$ when an energy measurement is made on this state?

(c) What is the probability of finding the value $5\hbar\omega_0/2$ when an energy measurement is made on this state?

(d) What is the probability of finding a value greater than $\hbar\omega_0$ when an energy measurement is made on this state?

(e) What is the expectation value of the energy for this state?

(f) If a measurement of energy yields $3\hbar\omega_0/2$ at time $t = 0$, what is the state of the oscillator after the measurement? What can be said about a subsequent energy measurement taken at $t > 0$ (assuming that the system remains undisturbed between measurements)?

Question D5

A particle in a one-dimensional harmonic oscillator well is represented at time t by the normalized wave packet

$$\Psi(x,t) = \frac{1}{\sqrt{6}}(\psi_0(x)\exp[-\mathrm{i}E_0t/\hbar] - 2\psi_1(x)\exp[-\mathrm{i}E_1t/\hbar] + \mathrm{i}\psi_3(x)\exp[-\mathrm{i}E_3t/\hbar]),$$

where $E_n = (n + \frac{1}{2})\hbar\omega_0$ and the $\psi_n(x)$ are orthonormal eigenfunctions. Determine the expectation value $\langle E\rangle$ and the uncertainty ΔE in this state, expressing your answers in terms of ω_0.

Question D6

A particle in a simple harmonic oscillator well with classical angular frequency ω_0 has an initial state represented by

$$\Psi(x,0) = N(2\psi_0(x) + \psi_1(x))$$

where the $\psi_n(x)$ are the normalized energy eigenfunctions with quantum numbers $n = 0$ and $n = 1$.

(a) Find the positive real value of the normalization constant N.

(b) Find the expectation value of the energy and the uncertainty in the energy for the state.

(c) At a time $t_1 > 0$ the energy of the particle in this state is measured. What is the probability that the value $\frac{1}{2}\hbar\omega_0$ is found?

(d) If an energy of $\frac{1}{2}\hbar\omega_0$ is found at time $t_1 > 0$, and the energy of the particle is measured again at time $t_2 > t_1$, what is the probability of finding the value $\frac{1}{2}\hbar\omega_0$ at time t_2?

Question D7

(a) Find the momentum amplitude $A(k)$ corresponding to the normalized free-particle wave packet

$$\Psi(x,0) = \left(\frac{1}{a\sqrt{\pi}}\right)^{1/2}\exp(-x^2/2a^2),$$

where $a > 0$ is a constant. You may use the integral

$$\int_{-\infty}^{\infty} \exp(-x^2/2a^2)\exp(-\mathrm{i}kx)\,\mathrm{d}x = \sqrt{2\pi}a\exp(-a^2k^2/2) \quad \text{for } a > 0.$$

(b) Use your answer to part (a) to estimate the probability of measuring a momentum in the range $-0.01\hbar/a \le \hbar k \le +0.01\hbar/a$, in the state described by $\Psi(x,0)$.

(c) Write down (but do not evaluate) an integral that gives the free-particle wave packet $\Psi(x,t)$ at any time $t > 0$.

E: Orbital angular momentum

Question E1

Which of the following functions, written in Cartesian coordinates (x,y) or plane polar coordinates (r,ϕ), are eigenfunctions of $\widehat{\mathrm{L}}_z$?

(i)	x	(ii)	xy
(iii)	x^2+y^2	(iv)	$x+\mathrm{i}y$
(v)	$(x-\mathrm{i}y)^2$	(vi)	$r^2\sin\phi$
(vii)	$r\mathrm{e}^{\mathrm{i}\phi}$	(viii)	$\mathrm{e}^{\mathrm{i}\phi}+\mathrm{e}^{-\mathrm{i}\phi}$

Question E2

(a) Write down the quantum-mechanical operator for L_z in 2D polar coordinates and find its eigenfunctions $\psi(r,\phi)$ and eigenvalues, using appropriate boundary conditions.

(b) Show that the eigenfunctions are mutually orthogonal.

At time $t = 0$, a particle moving in two dimensions is represented by the wave function

$$\psi(r,\phi) = AR(r)\sin(3\phi),$$

where A is a real positive constant and

$$\int_0^{\infty} |R(r)|^2\, r\,\mathrm{d}r = 1.$$

(c) Find the value of the constant A. You may use the standard integral $\int_0^{2\pi}\sin^2(3\phi)\,\mathrm{d}\phi = \pi$.

(d) Find the expectation value of L_z for the state $\psi(r,\phi)$ by using the sandwich rule.

(e) Express $\psi(r,\phi)$ as a linear combination of eigenfunctions of $\widehat{\mathrm{L}}_z$.

(f) What are the possible outcomes of a measurement of L_z on the state $\Psi(r,\phi)$, and what are their probabilities?

(g) Calculate the expectation value of L_z using your answers to part (f).

Question E3

In spherical coordinates the operator for the square of angular momentum is given by

$$\widehat{\mathrm{L}}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

(a) Show that this operator commutes with the operator for the z-component of angular momentum, and explain the significance of this.

(b) Show that the spherical harmonic function

$$Y_{l,m}(\theta,\phi) = A\sin(2\theta)\,\exp(\mathrm{i}\phi)$$

is an eigenfunction of both $\widehat{\mathrm{L}}_z$ and $\widehat{\mathrm{L}}^2$ and find the eigenvalues. What are the values of the quantum numbers m and l?

(c) Find the positive real value of the normalization constant A. You may use the standard integral

$$\int_0^{\pi}\sin^3\theta\cos^2\theta\,\mathrm{d}\theta = \tfrac{4}{15}.$$

Question E4

(a) Show that, for any operators, $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{B}}$,

$$\left[\widehat{\mathrm{A}}^2, \widehat{\mathrm{B}}\right] = \widehat{\mathrm{A}}\left[\widehat{\mathrm{A}}, \widehat{\mathrm{B}}\right] + \left[\widehat{\mathrm{A}}, \widehat{\mathrm{B}}\right]\widehat{\mathrm{A}}.$$

Given the operator

$$\widehat{\mathrm{L}}^2 = \widehat{\mathrm{L}}_x^2 + \widehat{\mathrm{L}}_y^2 + \widehat{\mathrm{L}}_z^2$$

and the commutation relations

$$[\widehat{\mathrm{L}}_x, \widehat{\mathrm{L}}_y] = \mathrm{i}\hbar\widehat{\mathrm{L}}_z,$$

$$[\widehat{\mathrm{L}}_y, \widehat{\mathrm{L}}_z] = \mathrm{i}\hbar\widehat{\mathrm{L}}_x,$$

$$[\widehat{\mathrm{L}}_z, \widehat{\mathrm{L}}_x] = \mathrm{i}\hbar\widehat{\mathrm{L}}_y,$$

between the operators for the components of angular momentum:

(b) Use the result of part (a) to show that $\widehat{\mathrm{L}}^2$ commutes with $\widehat{\mathrm{L}}_z$.

(c) What is the significance of the fact that the operators for the components of angular momentum do not commute with one another?

(d) What is the significance of the fact that the operators for the components of angular momentum commute with $\widehat{\mathrm{L}}^2$?

(e) Write down the operator for $\widehat{\mathrm{L}}_z$ in spherical coordinates and state its eigenfunctions and eigenvalues.

(f) What are the eigenvalues of $\widehat{\mathrm{L}}^2$ and how many different (technically, linearly independent) eigenfunctions have the same eigenvalue?

(g) Show that the function

$$\psi(\theta, \phi) = A \sin\theta\, \cos\phi$$

is an eigenfunction of $\widehat{\mathrm{L}}^2$ but not of $\widehat{\mathrm{L}}_z$. You may use the fact that

$$\widehat{\mathrm{L}}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

(h) Does the answer to part (f) conflict with the answer to part (c)?

(i) For a state $\psi(r, \theta, \phi) = R(r)\, \sin\theta\, \cos\phi$ what are the possible outcomes of a measurement of $\widehat{\mathrm{L}}_z$ and what are their probabilities?

(j) Describe the outcomes of measuring $\widehat{\mathrm{L}}_z$ and $\widehat{\mathrm{L}}^2$ for the state $\psi(r, \theta, \phi)$ given in part (i).

F: Spin angular momentum

Question F1

At a fixed time, the spin state of an electron is given by the normalized spinor

$$|A\rangle = \frac{1}{5^{1/2}}\begin{bmatrix}1\\2\mathrm{i}\end{bmatrix}.$$

The operator for the S_y observable is

$$\widehat{\mathrm{S}}_y = \frac{\hbar}{2}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix},$$

which has orthonormal eigenvectors

$$|\uparrow_y\rangle = \frac{1}{2^{1/2}}\begin{bmatrix}1\\ \mathrm{i}\end{bmatrix}, \quad |\downarrow_y\rangle = \frac{1}{2^{1/2}}\begin{bmatrix}\mathrm{i}\\ 1\end{bmatrix}$$

corresponding to the eigenvalues $S_y = \hbar/2$ and $S_y = -\hbar/2$ respectively.

(a) What is the probability that a measurement of S_y in the state $|A\rangle$ will yield the value $-\hbar/2$?

(b) What are the expectation values of S_y and S_y^2 in the state $|A\rangle$?

(c) Find ΔS_y in the state $|A\rangle$.

(d) The z-component of the spin of the electron is measured and found to be $-\hbar/2$. What is the spin state immediately after this measurement? Write this in terms of $|\uparrow_y\rangle$ and $|\downarrow_y\rangle$ as given above. What is the probability of getting the value $S_y = -\hbar/2$ if the y-component of spin is measured immediately after the above measurement?

Question F2

This question is about the precession of spin in an applied magnetic field. At $t = 0$ an electron is initially in an eigenstate of S_x with eigenvalue $\hbar/2$. The magnetic field has magnitude B and is directed along the z-axis.

(a) The matrix representing S_x is

$$\widehat{\mathrm{S}}_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Show that the initial eigenstate (with eigenvalue $S_x = \hbar/2$) can be represented by the spinor

$$|A\rangle_{\text{initial}} = \frac{1}{2^{1/2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

(b) The Hamiltonian matrix for spin evolution is

$$\widehat{\mathrm{H}} = \omega\widehat{\mathrm{S}}_z = \frac{\hbar\omega}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Show that the orthonormal spinors

$$|\uparrow_z\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |\downarrow_z\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

are eigenvectors of $\widehat{\mathrm{H}}$ with eigenvalues $E_{\mathrm{u}} = \hbar\omega/2$ and $E_{\mathrm{d}} = -\hbar\omega/2$, respectively.

(c) Express the initial spinor $|A\rangle_{\text{initial}}$ as a linear superposition of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ and hence write down the spinor $|A\rangle$ representing the spin state at a later time t.

(d) At time t the electron passes through a pair of Stern–Gerlach magnets to measure S_x. Find the probability (as a function of time) that it will be measured to have component $S_x = +\hbar/2$.

Question F3

Consider the evolution of the spin state of an electron (charge $-e$, mass m) in a magnetic field of magnitude B directed along the y-axis. The Hamiltonian matrix is

$$\widehat{\mathrm{H}} = \omega\widehat{\mathrm{S}}_y = \tfrac{1}{2}\hbar\omega\begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix},$$

and $\omega = eB/m$.

(a) Show that the spinors

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \mathrm{i} \end{bmatrix} \quad \text{and} \quad |\downarrow_y\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} \mathrm{i} \\ 1 \end{bmatrix}$$

are orthonormal.

(b) Verify that $|\uparrow_y\rangle$ and $|\downarrow_y\rangle$ are eigenvectors of $\widehat{\mathrm{H}}$, and find the corresponding eigenvalues E_{u} and E_{d}.

(c) The spin state of the electron at any time t is represented by the spinor

$$|A\rangle = a_{\mathrm{u}}\exp(-\mathrm{i}E_{\mathrm{u}}t/\hbar)|\uparrow_y\rangle + a_{\mathrm{d}}\exp(-\mathrm{i}E_{\mathrm{d}}t/\hbar)|\downarrow_y\rangle$$

where a_{u} and a_{d} are constant amplitudes. The initial state is

$$|A\rangle_{\text{initial}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

which is an eigenstate of $\widehat{\mathrm{S}}_z$ with eigenvalue $\frac{1}{2}\hbar$. Evaluate a_{u} and a_{d}.

(d) Calculate the probabilities that a measurement of S_z at time t will give the results $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$.

(e) Hence, or otherwise, show that the expectation value of measurements of S_z at time t is $\frac{1}{2}\hbar\cos(\omega t)$.

Question F4

In Question F3 above, we considered the spin state of an electron in a magnetic field of magnitude B in the y-direction, for which the Hamiltonian operator is $\widehat{\mathrm{H}} = \omega\widehat{\mathrm{S}}_y$, where $\omega = eB/m$.

(a) Use the generalized Ehrenfest theorem to show that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_x\rangle = \omega\langle S_z\rangle,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_y\rangle = 0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_z\rangle = -\omega\langle S_x\rangle.$$

(b) Hence show that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle S_z\rangle = -\omega^2\langle S_z\rangle.$$

(c) Given that the initial state is $\begin{bmatrix}1\\0\end{bmatrix}$, deduce the time evolution of $\langle S_z\rangle$. Is this answer consistent with the answer to Question F3 above?

Question F5

The spin operators are

$$\widehat{\mathrm{S}}_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix},$$
$$\widehat{\mathrm{S}}_y = \frac{\hbar}{2}\begin{bmatrix}0 & -\mathrm{i}\\\mathrm{i} & 0\end{bmatrix},$$
$$\widehat{\mathrm{S}}_z = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}.$$

(a) Show that

$$[\widehat{\mathrm{S}}_y, \widehat{\mathrm{S}}_z] = \mathrm{i}\hbar\widehat{\mathrm{S}}_x.$$

(b) Calculate the expectation values of S_x, S_y and S_z in the state represented by the spinor $5^{-1/2}\begin{bmatrix}1\\2\end{bmatrix}$.

(c) Calculate the uncertainties of S_x, S_y and S_z in the state represented by this spinor.

(d) Show that your answers to part (c) satisfy the generalized uncertainty relation

$$\Delta A\,\Delta B \geq \tfrac{1}{2}|\,\langle\,[\widehat{\mathrm{A}}, \widehat{\mathrm{B}}]\,\rangle\,|.$$

Note that there are three possible combinations of spin components here.

G: Dirac notation

Question G1

Write expressions for the following in (i) the general Dirac notation, (ii) the wave mechanics notation for a particle in one dimension and (iii) the spinor notation for a spin-$\frac{1}{2}$ particle:

(a) a ket vector;

(b) a bra vector;

(c) an inner product;

(d) the normalization condition;

(e) the expectation value of an observable O.

Question G2

Here are two equations from SM358 Book 2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{1}{\mathrm{i}\hbar}\langle\,[\widehat{\mathrm{A}},\widehat{\mathrm{H}}]\,\rangle,$$
$$\Delta A\,\Delta B \geq \tfrac{1}{2}|\,\langle\,[\widehat{\mathrm{A}},\widehat{\mathrm{B}}]\,\rangle|$$

(a) Translate these symbols into words and compile two dictionary entries, choosing suitable headings in each case.

(b) By expanding the commutators, show that

$$\left[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\widehat{\mathrm{C}}\right] = \widehat{\mathrm{B}}\left[\widehat{\mathrm{A}},\widehat{\mathrm{C}}\right] + \left[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\right]\widehat{\mathrm{C}}.$$

(c) Use the results of parts (a) and (b), find the product of uncertainties $\Delta x\,\Delta p_x$ and the derivatives $\mathrm{d}\langle x\rangle/\mathrm{d}t$ and $\mathrm{d}\langle p_x\rangle/\mathrm{d}t$ for a free particle moving in one dimension.

(d) Repeat part (c) for a particle bound in one dimension by the potential $V(x) = \frac{1}{2}Cx^2$.

Question G3

Use the expression for the time evolution of the expectation value of an observable, namely

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{1}{\mathrm{i}\hbar}\langle\,[\widehat{\mathrm{A}},\widehat{\mathrm{H}}]\,\rangle,$$

to show that:

(a) the expectation value of the energy is constant for any state;

(b) the expectation value of an observable whose operator commutes with the Hamiltonian operator of a system is constant for any state;

(c) the expectation value of any observable is constant for a stationary state.

Question G4

Suppose that the operator $\widehat{\mathrm{A}}$ for an observable A has a complete orthonormal set of eigenvectors $|\phi_n\rangle\quad(n = 1, 2, 3, \ldots)$ with corresponding eigenvalues λ_n.

(a) Write down, in Dirac notation, the expression for the expectation value of a measurement of A on any state Ψ.

(b) If any state $|\Psi\rangle$ is expanded as a linear combination of the eigenstates of A,

$$|\Psi\rangle = \sum_{i=1}^{\infty} a_i|\phi_i\rangle,$$

use the expression $\langle A\rangle = \langle\Psi|\widehat{\mathrm{A}}|\Psi\rangle$ to show that

$$\langle A\rangle = \sum_{i=1}^{\infty} |a_i|^2\lambda_i,$$

where λ_i is the eigenvalue corresponding to the eigenvector $|\phi_i\rangle$.

(c) Show that the coefficients a_n defined in part (b) are given by

$$a_n = \langle\phi_n|\Psi\rangle.$$

(d) Write down, in Dirac notation, the overlap rule giving the probability that a measurement of the observable A on any state $|\Psi\rangle$ yields the value λ_n. Show that this probability is equal to $|a_n|^2$.

(e) Are the answers to parts (b) and (d) consistent?

Question G5

(a) Write down the condition that an operator $\widehat{\mathrm{A}}$ is Hermitian in

(i) Dirac notation;

(ii) wave function notation for a particle in one dimension;

(iii) spinor notation for a spin-$\frac{1}{2}$ particle.

(b) Show that the operator $\widehat{\mathrm{p}}_x = -\mathrm{i}\hbar(\partial/\partial x)$ in wave function notation is Hermitian.

(c) Show that the operator

$$\widehat{\mathrm{S}}_y = \tfrac{1}{2}\hbar \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}$$

in spinor notation is Hermitian.

Question G6

Prove, using Dirac notation, that:

(a) the eigenvalues of a Hermitian operator are real;

(b) the eigenvectors of a Hermitian operator corresponding to different eigenvalues are orthogonal;

(c) the expectation value of an observable represented by a Hermitian operator is real for any state.

H: Three-dimensional systems

Question H1

Consider an isotropic two-dimensional harmonic oscillator defined by the potential energy function $\frac{1}{2}C(x^2 + y^2) = \frac{1}{2}Cr^2$. An excited state of the oscillator is represented by the normalized energy eigenfunction

$$\psi(r, \phi) = A\mathrm{e}^{-\mathrm{i}\phi}\, r \exp(-r^2/2a^2)$$

where a is a positive constant and (r, ϕ) are plane polar coordinates.

(a) Find the real positive normalization constant A. You may use the standard integral

$$\int_0^\infty u^3 \exp(-u^2)\,\mathrm{d}u = \frac{1}{2}.$$

(b) Determine the expectation values $\langle L_z \rangle$ and $\langle L_z^2 \rangle$, and the uncertainty ΔL_z.

(c) What can you conclude about the outcome of a measurement of L_z on an oscillator in this state?

Question H2

In spherical coordinates, the ground-state energy eigenfunction of a three-dimensional system is given by

$$\psi(r, \theta, \phi) = (1/a\sqrt{\pi})^{3/2} \exp(-r^2/2a^2)$$

where $r = (x^2 + y^2 + z^2)^{1/2}$, and a is a positive constant. You may use the standard integrals

$$\int_0^\infty u^3 \exp(-u^2)\,\mathrm{d}u = \frac{1}{2} \quad \text{and} \quad \int_0^\infty u^4 \exp(-u^2)\,\mathrm{d}u = \frac{3}{8}\sqrt{\pi}.$$

(a) Calculate the expectation value $\langle r \rangle$ for this state.

(b) Evaluate $\langle r^2 \rangle$, and hence find the uncertainty Δr.

Question H3

(a) Write down the time-independent Schrödinger equation and the boundary conditions for a particle of mass m in a three-dimensional cubic box of side L with perfectly impenetrable walls, having one corner at the origin, and the opposite corner at the point (L, L, L).

(b) Show that

$$\psi(x, y, z) = A\sin(k_x x)\,\sin(k_y y)\,\sin(k_z z)$$

is a solution for certain values of k_x, k_y and k_z, and find the energy eigenvalues.

(c) Suppose that the state at time $t = 0$ is described by the normalized wave function

$$\Psi(x, y, z, 0) = \frac{4}{L^{3/2}}\sin(\pi x/L)\,\sin(2\pi y/L)\,\sin(2\pi z/L)\,\cos(4\pi z/L).$$

(i) What are the possible outcomes of a measurement of energy on the state, and what are their respective probabilities? You may use the identity

$$\sin B\,\cos C = \frac{1}{2}\left(\sin(B + C) + \sin(B - C)\right).$$

(ii) Find $\Psi(x, y, z, t)$.

Question H4

(a) Write down the time-independent Schrödinger equation for the hydrogen atom (consisting of an electron charge $-e$ and mass m) in terms of the Laplacian operator ∇^2. You may assume that the nucleus is very massive and is at the origin, and that the reduced mass is equal to m.

(b) In spherical coordinates,

$$\nabla^2 = \frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r + \text{terms containing derivatives with respect to } \theta \text{ and } \phi.$$

Express the time-independent Schrödinger equation for spherically symmetric solutions $\psi(r)$ as a differential equation with independent variable r.

(c) Show that

$$\psi(r) = A\exp(-\lambda r)$$

is a solution if $\lambda = \dfrac{me^2}{4\pi\varepsilon_0\hbar^2}$ and find the energy of the state in terms of m and e.

(d) Find a value of A which normalizes $\psi(r)$. You may use the standard integral

$$\int_0^\infty u^n \mathrm{e}^{-u}\,\mathrm{d}u = n! \quad \text{for } n = 0, 1, 2, \ldots.$$

Answers

A: Schrödinger's equation

Answer A1

(a) The appropriate Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = \mathrm{i}\hbar\frac{\partial\Psi}{\partial t}.$$

(b) Partially differentiating $\Psi(x,t) = A\exp(\mathrm{i}(kx-\omega t))$ twice with respect to x, and once with respect to t gives

$$\frac{\partial\Psi}{\partial x} = \mathrm{i}kA\exp(\mathrm{i}(kx-\omega t))$$

$$\frac{\partial^2\Psi}{\partial x^2} = (\mathrm{i}k)^2 A\exp(\mathrm{i}(kx-\omega t)) = -k^2\Psi(x,t)$$

$$\frac{\partial\Psi}{\partial t} = -\mathrm{i}\omega A\exp(\mathrm{i}(kx-\omega t)) = -\mathrm{i}\omega\Psi(x,t).$$

Substituting these results into the Schrödinger equation of part (a) gives

$$\frac{\hbar^2k^2}{2m}\Psi(x,t) = \mathrm{i}\hbar\left(-\mathrm{i}\omega\Psi(x,t)\right) = \hbar\omega\Psi(x,t).$$

So the given function obeys Schrödinger's equation, provided that

$$\omega = \frac{\hbar k^2}{2m}.$$

Answer A2

Schrödinger's equation is

$$\widehat{\mathrm{H}}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\,\Psi(x,t) = \mathrm{i}\hbar\frac{\partial\Psi}{\partial t}.$$

Substituting $\Psi(x,t) = \psi(x)\,T(t)$ into both sides of this equation gives

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\,\psi(x)\right)T(t) = \mathrm{i}\hbar\frac{\mathrm{d}T}{\mathrm{d}t}\,\psi(x).$$

Using the time-independent Schrödinger equation, we then get

$$E\psi(x)\,T(t) = \mathrm{i}\hbar\frac{\mathrm{d}T}{\mathrm{d}t}\,\psi(x),$$

so

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{-\mathrm{i}E}{\hbar}\,T(t).$$

This equation has the solution

$$T(t) = A\exp(-\mathrm{i}Et/\hbar),$$

where A is a constant, as can be confirmed by differentiating both sides with respect to t.

B: The time-independent Schrödinger equation

Answer B1

(a) The appropriate time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi(x) \quad \text{for } -a \le x \le a.$$

The energy eigenfunction $\psi(x)$ is zero outside the well and must be continuous everywhere, so the associated boundary conditions are:

$$\psi(a) = 0 \quad \text{and} \quad \psi(-a) = 0.$$

There is no boundary condition for $\psi'(x)$ at $x = \pm a$ because the potential energy function goes to infinity at these points.

(b) Inside the well, we obtain

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[A\cos\left(\frac{5\pi x}{2a}\right)\right] = -\left(\frac{5\pi}{2a}\right)^2 A\cos\left(\frac{5\pi x}{2a}\right) = -\left(\frac{5\pi}{2a}\right)^2 \psi(x).$$

Substituting into the time-independent Schrödinger equation gives

$$\frac{\hbar^2}{2m}\left(\frac{5\pi}{2a}\right)^2 \psi(x) = E\psi(x),$$

so the given function satisfies the equation provided that

$$E = \frac{\hbar^2}{2m}\left(\frac{5\pi}{2a}\right)^2 = \frac{25\hbar^2\pi^2}{8ma^2}.$$

Also, the given function satisfies the associated boundary conditions $\psi(\pm a) = A\cos(\pm 5\pi/2) = 0$.

(c) The normalization condition requires that

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x = \int_{-a}^{a} |A|^2 \cos^2\left(\frac{5\pi x}{2a}\right) \mathrm{d}x = |A|^2 \int_{-a}^{a} \cos^2\left(\frac{5\pi x}{2a}\right) \mathrm{d}x.$$

To carry out the integral, we make the substitution $u = 5\pi x/2a$. Then $x = (2a/5\pi)u$ and $\mathrm{d}x = (2a/5\pi)\,\mathrm{d}u$. The limits $x = \pm a$ become $u = \pm 5\pi/2$, so

$$\begin{aligned} 1 &= |A|^2 \int_{-5\pi/2}^{5\pi/2} \cos^2 u \cdot \frac{2a}{5\pi}\,\mathrm{d}u = \frac{2a}{5\pi}|A|^2 \int_{-5\pi/2}^{5\pi/2} \cos^2 u \,\mathrm{d}u \\ &= \frac{2a}{5\pi}|A|^2 \times \frac{5\pi}{2} = a|A|^2. \end{aligned}$$

Hence $|A|^2 = 1/a$. Assuming that A is real and positive, $A = 1/\sqrt{a}$.

(d) The probability of finding the particle in the given interval is

$$\text{Probability} = \int_{-0.2a}^{0.2a} |\psi(x)|^2 \,\mathrm{d}x = \frac{1}{a}\int_{-0.2a}^{0.2a} \cos^2\left(\frac{5\pi x}{2a}\right) \mathrm{d}x$$

Making once again the substitution $u = 5\pi x/2a$, the limits $x = \pm 0.2a$ become $u = \pm\pi/2$, so

$$\begin{aligned} \text{Probability} &= \frac{1}{a}\int_{-\pi/2}^{\pi/2} \cos^2 u \cdot \frac{2a}{5\pi}\,\mathrm{d}u = \frac{2}{5\pi}\int_{-\pi/2}^{\pi/2} \cos^2 u \,\mathrm{d}u \\ &= \frac{2}{5\pi} \times \frac{\pi}{2} = \frac{1}{5}. \end{aligned}$$

Answer B2

(a)

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi(x), \quad \text{for } 0 \le x \le L.$$

(b) Differentiating the function

$$\psi(x) = A\sin[(2mE)^{1/2}x/\hbar] + B\cos[(2mE)^{1/2}x/\hbar]$$

gives

$$\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} = \frac{(2mE)^{1/2}}{\hbar}A\cos[(2mE)^{1/2}x/\hbar] - \frac{(2mE)^{1/2}}{\hbar}B\sin[(2mE)^{1/2}x/\hbar],$$

and differentiating again,

$$\begin{aligned}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} &= -\frac{2mE}{\hbar^2}A\sin[(2mE)^{1/2}x/\hbar] - \frac{2mE}{\hbar^2}B\cos[(2mE)^{1/2}x/\hbar] \\ &= -\frac{2mE}{\hbar^2}\psi(x).\end{aligned}$$

Hence

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{\hbar^2}{2m}\frac{2mE}{\hbar^2}\psi(x) = E\psi(x),$$

and so the function satisfies the time-independent Schrödinger equation.

(c) The boundary conditions are $\psi(0) = 0$ and $\psi(L) = 0$. The boundary condition $\psi(0) = 0$ gives $B = 0$. The condition $\psi(L) = 0$ gives

$$A\sin\left(\frac{(2mE)^{1/2}L}{\hbar}\right) = 0.$$

For a non-trivial solution, $A \neq 0$ and so

$$\frac{(2mE)^{1/2}L}{\hbar} = n\pi,$$

where n is an integer. So

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2},$$

where n is an integer. So the solution for $\psi(x)$ is

$$\psi(x) = A\sin\left(\frac{n\pi x}{L}\right).$$

The case $n = 0$ corresponds to the trivial solution $\psi(x) = 0$, and can be ignored. Any negative integer $-n$ gives the same solution as $+n$ (apart from an irrelevant phase factor of -1), so we can restrict n to the positive integers: $n = 1, 2, 3, \ldots$.

(d) The normalization condition gives

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2\,\mathrm{d}x = \int_0^L |A|^2\sin^2\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x,$$

since $\psi(x) = 0$ for $x < 0$ and for $x > L$. Make the substitution $u = n\pi x/L$. Then $\mathrm{d}x = (L/n\pi)\,\mathrm{d}u$ and the limits of integration become $u = 0$ and $u = n\pi$. Using the given standard integral, we then obtain

$$\begin{aligned}1 &= |A|^2\frac{L}{n\pi}\int_0^{n\pi}\sin^2 u\,\mathrm{d}u \\ &= |A|^2\frac{L}{n\pi}\times\left[\frac{1}{2}u - \frac{1}{4}\sin 2u\right]_{u=0}^{u=n\pi} \\ &= \frac{|A|^2L}{2}.\end{aligned}$$

Hence $|A|^2 = 2/L$. Taking A to be real and positive, $A = \sqrt{2/L}$.

(e) The second excited state corresponds to $n = 3$ and the corresponding stationary-state wave function is

$$\Psi_3(x,t) = \psi_3(x)\exp(-\mathrm{i}E_3t/\hbar) = \sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)\exp\left(-\mathrm{i}\frac{9\pi^2\hbar t}{2mL^2}\right).$$

(f) The probability density function is

$$|\Psi_3(x,t)|^2 = \frac{2}{L}\sin^2\left(\frac{3\pi x}{L}\right).$$

So the required probability P is

$$P = \int_0^{L/9}|\psi(x)|^2\,\mathrm{d}x = \frac{2}{L}\int_0^{L/9}\sin^2\left(\frac{3\pi x}{L}\right)\,\mathrm{d}x.$$

We make the substitution $u = 3\pi x/L$. Then $\mathrm{d}x = (L/3\pi)\,\mathrm{d}u$ and the limits of integration become $u = 0$ and $u = \pi/3$. Hence

$$\begin{aligned}
P &= \frac{2}{L}\frac{L}{3\pi}\int_0^{\pi/3} \sin^2 u \,\mathrm{d}u \\
&= \frac{2}{3\pi}\left[\frac{1}{2}u - \frac{1}{4}\sin(2u)\right]_{u=0}^{u=\pi/3} = \frac{2}{3\pi}\left[\frac{\pi}{6} - \frac{1}{4}\sin\left(\frac{2\pi}{3}\right)\right] \\
&= \frac{1}{9} - \frac{\sqrt{3}}{12\pi} = 0.0652.
\end{aligned}$$

Answer B3

(a) The appropriate time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}Cx^2\,\psi(x) = E\psi(x).$$

(b) Differentiating $\psi = x\exp[-x^2/2a^2]$ with respect to x, we get

$$\begin{aligned}
\psi'(x) &= 1 \times \exp[-x^2/2a^2] + x\left(\frac{-x}{a^2}\right)\exp[-x^2/2a^2] \\
&= \left(1 - \frac{x^2}{a^2}\right)\exp[-x^2/2a^2].
\end{aligned}$$

Differentiating again,

$$\begin{aligned}
\psi'' &= -\frac{2x}{a^2}\exp[-x^2/2a^2] + \left(1 - \frac{x^2}{a^2}\right)\left(\frac{-x}{a^2}\right)\exp[-x^2/2a^2] \\
&= \left(-\frac{3x}{a^2} + \frac{x^3}{a^4}\right)\exp[-x^2/2a^2].
\end{aligned}$$

Substituting into the time-independent Schrödinger equation we get

$$-\frac{\hbar^2}{2m}\left(-\frac{3x}{a^2} + \frac{x^3}{a^4}\right)\exp[-x^2/2a^2] + \frac{1}{2}Cx^3\exp[-x^2/2a^2] = Ex\exp[-x^2/2a^2].$$

Dividing through by $\exp[-x^2/2a^2]$ then gives

$$-\frac{\hbar^2}{2m}\left(-\frac{3x}{a^2} + \frac{x^3}{a^4}\right) + \frac{1}{2}Cx^3 = Ex.$$

Equating the coefficients of x^3 on both sides gives

$$-\frac{\hbar^2}{2ma^4} + \frac{C}{2} = 0 \quad \text{so} \quad \frac{\hbar^2}{2ma^4} = \frac{C}{2} \quad \text{and} \quad a^2 = \frac{\hbar}{\sqrt{mC}}.$$

Equating coefficients of x on both sides then gives

$$E = \frac{3\hbar^2}{2ma^2} = \frac{3}{2}\hbar\sqrt{\frac{C}{m}} = \frac{3}{2}\hbar\omega_0.$$

(c) We introduce a normalization constant A so that $\psi(x) = Ax\exp[-x^2/2a^2]$. Then the normalization condition gives

$$1 = |A|^2\int_{-\infty}^{+\infty} x^2\exp(-x^2/a^2)\,\mathrm{d}x.$$

We change the variable of integration to $u = x/a$. Then $\mathrm{d}x = a\,\mathrm{d}u$ and the limits of integration become $u = \pm\infty$. Hence

$$1 = |A|^2a^3\int_{-\infty}^{\infty} u^2\exp(-u^2)\,\mathrm{d}u = |A|^2a^3\frac{\sqrt{\pi}}{2}.$$

Choosing A to be real and positive,

$$A = \left(\frac{2}{a^3\pi^{1/2}}\right)^{1/2}.$$

Recalling that $E = 3\hbar\omega_0/2$, the corresponding normalized stationary-state wave function is

$$\Psi(x,t) = \left(\frac{2}{a^3\pi^{1/2}}\right)^{1/2} x \exp\left(-\frac{x^2}{2a^2}\right) \exp\left(-\tfrac{3}{2}\mathrm{i}\omega_0 t\right).$$

Answer B4

(a) The appropriate time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}Cx^2\,\psi(x) = E\psi(x).$$

(b) Differentiating $\psi(x) = A\exp(-x^2/2a^2)$ once,

$$\psi'(x) = -A\frac{x}{a^2}\exp(-x^2/2a^2),$$

and differentiating again,

$$\begin{aligned}\psi''(x) &= -A\frac{1}{a^2}\exp(-x^2/2a^2) - A\frac{x}{a^2}\left(\frac{-x}{a^2}\right)\exp(-x^2/2a^2)\\ &= A\left(\frac{x^2}{a^4} - \frac{1}{a^2}\right)\exp(-x^2/2a^2).\end{aligned}$$

Substituting into the time-independent Schrödinger equation, and cancelling the factor $A\exp(-x^2/2a^2)$, we obtain

$$-\frac{\hbar^2}{2m}\left(\frac{x^2}{a^4} - \frac{1}{a^2}\right) + \frac{1}{2}Cx^2 = E.$$

Equating terms in x^2 gives

$$-\frac{\hbar^2}{2ma^4} + \frac{1}{2}C = 0 \quad \text{so} \quad \frac{\hbar^2}{2ma^4} = \frac{1}{2}C \quad \text{and} \quad a^2 = \frac{\hbar}{\sqrt{mC}},$$

as required. Equating the constant terms gives

$$E = \frac{\hbar^2}{2ma^2} = \frac{\hbar}{2}\sqrt{\frac{C}{m}}.$$

The classical angular frequency is

$$\omega_0 = \sqrt{\frac{C}{m}}.$$

So

$$E = \frac{1}{2}\hbar\omega_0.$$

(c) The normalization condition is

$$1 = \int_{-\infty}^{\infty}|\psi(x)|^2\,\mathrm{d}x = |A|^2\int_{-\infty}^{\infty}\exp(-x^2/a^2)\,\mathrm{d}x$$

We make the substitution $u = x/a$. Then $\mathrm{d}x = a\,\mathrm{d}u$ and the limits of integration become $u = \pm\infty$. So

$$1 = |A|^2 a\int_{-\infty}^{\infty}\exp(-u^2)\,\mathrm{d}u = |A|^2 a\sqrt{\pi}.$$

Taking A to be real and positive, we get

$$A = \left(\frac{1}{a\sqrt{\pi}}\right)^{1/2}.$$

(d) The function $\psi(x)$ is even because

$$\psi(-x) = A\exp(-(-x)^2/a^2) + A\exp(-x^2/a^2) = \psi(x)$$

for all x.

(e) In classical physics, the particle is confined to the region where the kinetic energy is positive or zero. If the kinetic energy is zero at $x = d$, then the total energy E is equal to the potential energy, $\frac{1}{2}Cd^2$. So a classical particle with energy E is confined to the region $-d \leq x \leq d$, where $E = \frac{1}{2}\hbar\omega_0 = \frac{1}{2}Cd^2$. So

$$d^2 = \frac{\hbar\omega_0}{C} = \frac{\hbar}{\sqrt{mC}} = a^2.$$

So a classical particle with energy $E = \frac{1}{2}\hbar\omega_0$ is confined to the region $-a \leq x \leq a$.

(f) The quantum mechanical probability is

$$\text{Probability} = |A|^2 \int_{-a}^{a} \exp(-x^2/a^2)\,\mathrm{d}x = \frac{1}{a\sqrt{\pi}} \int_{-a}^{a} \exp(-x^2/a^2)\,\mathrm{d}x.$$

We change the variable of integration to $u = x/a$. Then $\mathrm{d}x = a\,\mathrm{d}u$ and the limits of integration become $u = \pm 1$. So

$$\begin{aligned}\text{Probability} &= \frac{1}{a\sqrt{\pi}}\, a \int_{u=-1}^{u=1} \exp(-u^2)\,\mathrm{d}u = \frac{2}{\sqrt{\pi}} \int_{u=0}^{u=1} \exp(-u^2)\,\mathrm{d}u \\ &= \frac{2}{\sqrt{\pi}} \times 0.747 = 0.843.\end{aligned}$$

C: Eigenfunctions, expectation values and uncertainties

Answer C1

(a) The normalization condition gives

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2\,\mathrm{d}x = \frac{4N^2}{a^2} \int_{-\infty}^{\infty} x^2 \exp(-x^2/a^2)\,\mathrm{d}x.$$

We change the variable of integration to $u = x/a$. Then $\mathrm{d}x = a\,\mathrm{d}u$ and the limits of integration become $u = \pm\infty$. So

$$1 = \frac{4N^2}{a^2} a^3 \int_{-\infty}^{\infty} u^2 \exp(-u^2)\,\mathrm{d}u = 2N^2 a\sqrt{\pi}.$$

Choosing N to be real and positive we have

$$N = \left(\frac{1}{2a\sqrt{\pi}}\right)^{1/2}.$$

(b) We have

$$\psi(-x) = N\left(\frac{-2x}{a}\right)\exp(-(-x)^2/2a^2) = -N\left(\frac{2x}{a}\right)\exp(-x^2/2a^2) = -\psi(x)$$

so the energy eigenfunction $\psi(x)$ is an odd function (which is consistent with it being the first excited state in a symmetrical well).

The expectation value of x is

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2\,\mathrm{d}x.$$

This is equal to zero because the integrand is odd and the range of integration is centred on $x = 0$. The oddness of the integrand follows because $|\psi(x)|^2$ is even and x is odd: we have odd $\times$ even $=$ odd.

The expectation value of p_x is

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^*(x)(-\mathrm{i}\hbar)\frac{\mathrm{d}\psi}{\mathrm{d}x}\,\mathrm{d}x.$$

This is equal to zero because the integrand is odd and the range of integration is centred on $x = 0$. The oddness of the integrand follows because $\psi(x)$ and $\psi^*(x)$ are odd functions and $\mathrm{d}/\mathrm{d}x$ is an odd operator: we have odd $\times$ odd $\times$ odd $=$ odd. (Alternatively, differentiation of $\psi(x)$ shows that $\mathrm{d}\psi/\mathrm{d}x$ is even, and odd $\times$ even $=$ odd).

(c) The expectation value of x^2 is

$$\langle x^2 \rangle = \frac{4N^2}{a^2}\int_{-\infty}^{\infty} x^4 \exp\left(-\frac{x^2}{a^2}\right)\mathrm{d}x.$$

We make the substitution $u = x/a$. Then $\mathrm{d}x = a\,\mathrm{d}u$ and the limits of integration become $u = \pm\infty$. So

$$\begin{aligned}\langle x^2 \rangle &= \frac{4N^2}{a^2}\,a^5\int_{-\infty}^{\infty} u^4\exp(-u^2)\,\mathrm{d}u = (4N^2a^3)\left(\frac{3}{4}\sqrt{\pi}\right)\\ &= 3\sqrt{\pi}\,a^3\,N^2 = \frac{3}{2}\,a^2.\end{aligned}$$

So the uncertainty in x is

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = (3/2)^{1/2}\;a.$$

Answer C2

(a) Because the eigenfunctions $\psi_n(x)$ are either even or odd functions of x, the corresponding stationary states $\Psi_n(x,t) = \psi_n(x)\exp(-\mathrm{i}E_nt/\hbar)$ are also either even or odd functions of x.

In a stationary state,

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi_n^*(x,t)\,x\,\Psi_n(x,t)\,\mathrm{d}x = 0$$

because the integrand is an odd function and the range of integration is centred on $x = 0$. The integrand is odd because it is either the product of three odd functions (for odd eigenfunctions) or it is the product of one odd function and two even functions (for even eigenfunctions).

Similarly,

$$\langle p_x \rangle = -\mathrm{i}\hbar\int_{-\infty}^{\infty}\psi_n^*(x)\,\psi_n'(x)\,\mathrm{d}x = 0,$$

because the integrand is odd and the range of integration is centred on $x = 0$. The integrand is odd because differentiating an odd function produces an even function and vice versa, so the integrand is the product of an odd function and an even function, which is odd.

(b) For the stationary state $\Psi_n(x,t) = \psi_n(x)\exp(-\mathrm{i}E_nt/\hbar)$:

$$\langle A \rangle = \int_{-\infty}^{\infty}\psi_n^*(x)\exp(\mathrm{i}E_nt/\hbar)\,\widehat{\mathrm{A}}\,\psi_n(x)\;\exp(-\mathrm{i}E_nt/\hbar)\,\mathrm{d}x = \int_{-\infty}^{\infty}\psi_n^*(x)\,\widehat{\mathrm{A}}\,\psi_n(x)\,\mathrm{d}x,$$

which is independent of time.

(c) For the stationary state $\Psi_n(x,t) = \psi_n(x)\;\exp(-\mathrm{i}E_nt/\hbar)$, with energy eigenvalue E_n

$$\begin{aligned}\langle E \rangle &= \int_{-\infty}^{\infty}\psi_n^*(x)\,\widehat{\mathrm{H}}\,\psi_n(x)\,\mathrm{d}x\\ &= \int_{-\infty}^{\infty}\psi_n^*(x)\,E_n\,\psi_n(x)\,\mathrm{d}x\\ &= E_n\int_{-\infty}^{\infty}\psi_n^*(x)\,\psi_n(x)\,\mathrm{d}x = E_n.\end{aligned}$$

Similarly:

$$\begin{aligned}\langle E^2\rangle &= \int_{-\infty}^{\infty} \psi_n^*(x)\,\widehat{\mathrm{H}}^2\,\psi_n(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \psi_n^*(x)\,E_n^2\,\psi_n(x)\,\mathrm{d}x \\ &= E_n^2 \int_{-\infty}^{\infty} \psi_n^*(x)\,\psi_n(x)\,\mathrm{d}x = E_n^2.\end{aligned}$$

Hence $\Delta E = (\langle E^2\rangle - \langle E\rangle^2)^{1/2} = (E_n^2 - E_n^2)^{1/2} = 0$. This expresses the fact that an energy measurement for a stationary state has a definite outcome.

(d) For a *real* wave function ψ:

$$\langle p_x\rangle = -\mathrm{i}\hbar \int_{-\infty}^{\infty} \psi^* \frac{\mathrm{d}\psi}{\mathrm{d}x}\,\mathrm{d}x = -\mathrm{i}\hbar \int_{-\infty}^{\infty} \psi \frac{\mathrm{d}\psi}{\mathrm{d}x}\,\mathrm{d}x.$$

Using the identity given in the question,

$$\langle p_x\rangle = -\left(\frac{\mathrm{i}\hbar}{2}\right) \int_{-\infty}^{\infty} \frac{\mathrm{d}\psi^2}{\mathrm{d}x}\,\mathrm{d}x = -\left(\frac{1}{2}\mathrm{i}\hbar\right)\left[\psi^2\right]_{x=-\infty}^{x=\infty} = 0,$$

since ψ must vanish as $x \to \pm\infty$.

Answer C3

(a)

$$\begin{aligned}-\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{(2\pi)^{1/2}}\exp(\mathrm{i}k_x x) &= \hbar k_x \frac{1}{(2\pi)^{1/2}}\exp(\mathrm{i}k_x x) \\ &= p_x\,\frac{1}{(2\pi)^{1/2}}\exp(\mathrm{i}k_x x),\end{aligned}$$

where $p_x = \hbar k_x$.

(b) The free particle Hamiltonian operator is

$$\widehat{\mathrm{H}} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

and the corresponding eigenvalue equation is

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_{k_x}(x) &= -\frac{\hbar^2}{2m}(\mathrm{i}k_x)^2\psi_{k_x}(x) = \frac{\hbar^2 k_x^2}{2m}\,\psi_{k_x}(x) \\ &= E\,\psi_{k_x}(x),\end{aligned}$$

where $E = \hbar^2 k_x^2/2m$. This energy eigenvalue is doubly degenerate because $+|k_x|$ and $-|k_x|$ both give the same energy. Classically, this degeneracy corresponds to particles travelling to the right and left with the same speed.

(c) The eigenfunction $\psi_{k_x}(x)$ cannot be normalized. We resolve this by forming normalizable linear superpositions over the continuum of momentum eigenfunctions.

Answer C4

(a) The expectation value of x is given by the sandwich integral

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi_2^*(x)\,x\,\psi_2(x)\,\mathrm{d}x = \frac{2}{L}\int_{-L/2}^{L/2} x\sin^2(2\pi x/L)\,\mathrm{d}x = 0$$

because the integrand is a odd function and the range of integration is centred on $x = 0$. (Note that the limits of integration change from $\pm\infty$ in the general case to $\pm L/2$ in this particular case because $\psi_2(x)$ vanishes outside the well.)

The expectation value of x^2 is given by

$$\langle x^2\rangle = \int_{-\infty}^{\infty} \psi_2^*(x)\,x^2\,\psi_2(x)\,\mathrm{d}x = \frac{2}{L}\int_{-L/2}^{L/2} x^2\sin^2(2\pi x/L)\,\mathrm{d}x = 0.$$

We make the substitution $u = 2\pi x/L$. Then, $\mathrm{d}x = (L/2\pi)\,\mathrm{d}u$ and the limits of integration become $u = \pm\pi$. Hence

$$\begin{aligned}\langle x^2\rangle &= \frac{2}{L}\left(\frac{L}{2\pi}\right)^3 \int_{-\pi}^{\pi} u^2 \sin^2 u\,\mathrm{d}u = \frac{L^2}{4\pi^3}\int_{-\pi}^{\pi} u^2\,\sin^2 u\,\mathrm{d}u \\ &= \frac{L^2}{4\pi^3}\left[\frac{\pi^3}{3} - \frac{\pi}{2}\right] = \left[\frac{1}{12} - \frac{1}{8\pi^2}\right] L^2 = 0.0707\,L^2.\end{aligned}$$

Therefore

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = 0.0707L^2$$

and

$$\Delta x = \sqrt{0.0707}\,L = 0.266L.$$

(b) The expectation value of p_x is given by the sandwich integral

$$\begin{aligned}\langle p_x\rangle &= \frac{2}{L}\int_{-L/2}^{L/2} \sin\left(\frac{2\pi x}{L}\right)\left(-\mathrm{i}\hbar\frac{\partial}{\partial x}\right)\sin\left(\frac{2\pi x}{L}\right)\,\mathrm{d}x \\ &= -\mathrm{i}\hbar\frac{2}{L}\,\frac{2\pi}{L}\int_{-L/2}^{L/2} \sin\left(\frac{2\pi x}{L}\right)\,\cos\left(\frac{2\pi x}{L}\right)\,\mathrm{d}x \\ &= 0,\end{aligned}$$

because the integrand is odd and the range of integration is symmetric about $x = 0$.

The expectation value of p_x^2 is

$$\begin{aligned}\langle p_x^2\rangle &= \frac{2}{L}\int_{-L/2}^{+L/2} \sin(2\pi x/L)(-\hbar^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sin(2\pi x/L)\,\mathrm{d}x \\ &= \frac{2\hbar^2}{L}\left(\frac{2\pi}{L}\right)^2\int_{-L/2}^{+L/2}\sin^2(2\pi x/L)\,\mathrm{d}x.\end{aligned}$$

We make the substitution $u = 2\pi x/L$. Then $\mathrm{d}x = (L/2\pi)\,\mathrm{d}u$ and the limits of integration become $u = \pm\pi$. So we have

$$\begin{aligned}\langle p_x^2\rangle &= \frac{2\hbar^2}{L}\left(\frac{2\pi}{L}\right)^2\frac{L}{2\pi}\int_{-\pi}^{\pi}\sin^2 u\,\mathrm{d}u = \frac{2\hbar^2}{L}\left(\frac{2\pi}{L}\right)\pi \\ &= \frac{4\hbar^2\pi^2}{L^2}.\end{aligned}$$

Therefore $\Delta p_x = \left(\langle p_x^2\rangle - \langle p_x\rangle^2\right)^{1/2} = 2\hbar\pi/L$.

(c) We have $\Delta p_x\,\Delta x = (2\hbar\pi/L)(0.266L) = 1.67\hbar$, which agrees with the uncertainty principle, $\Delta p_x\,\Delta x \geq \hbar/2$.

D: Wave packets

Answer D1

(a) The expectation value is given by

$$\langle x\rangle = \frac{a}{\sqrt{2}}\int_{-\infty}^{\infty}\psi^*(x)\left(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger\right)\psi(x)\,\mathrm{d}x.$$

We have

$$\begin{aligned}\widehat{\mathrm{A}}\psi(x) &= \widehat{\mathrm{A}}[c_0\psi_0(x) + c_1\psi_1(x) + c_2\psi_2(x)] \\ &= c_1\psi_0(x) + \sqrt{2}c_2\psi_1(x).\end{aligned}$$

So, using orthonormality,

$$\int_{-\infty}^{\infty} \psi^*(x)\,\widehat{\mathrm{A}}\,\psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} [c_0\psi_0(x) + c_1\psi_1(x) + c_2\psi_2(x)]^*[c_1\psi_0(x) + \sqrt{2}c_2\psi_1(x)]\,\mathrm{d}x$$
$$= c_0^*c_1 + \sqrt{2}c_1^*c_2.$$

Similarly,

$$\widehat{\mathrm{A}}^\dagger\psi(x) = \widehat{\mathrm{A}}^\dagger[c_0\psi_0(x) + c_1\psi_1(x) + c_2\psi_2(x)]$$
$$= c_0\psi_1(x) + \sqrt{2}c_1\psi_2(x) + \sqrt{3}c_2\psi_3(x).$$

So

$$\int_{-\infty}^{\infty} \psi^*(x)\,\widehat{\mathrm{A}}^\dagger\,\psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} [c_0\psi_0(x) + c_1\psi_1(x) + c_2\psi_2(x)]^*[c_0\psi_1(x) + \sqrt{2}c_1\psi_2(x) + \sqrt{3}c_2\psi_3(x)]\,\mathrm{d}x$$
$$= c_1^*c_0 + \sqrt{2}c_2^*c_1.$$

We therefore obtain

$$\langle x\rangle = \frac{a}{\sqrt{2}}\left(c_0^*c_1 + c_1^*c_0 + \sqrt{2}(c_1^*c_2 + c_2^*c_1)\right)$$
$$= a\left(\sqrt{2}\,\mathrm{Re}(c_0^*c_1) + 2\,\mathrm{Re}(c_1^*c_2)\right).$$

(b) In the special case where $c_1 = 0$, we have $\langle x\rangle = 0$.

(c) In the special case where $c_0 = 1/\sqrt{2}$, $c_1 = 1/\sqrt{2}$ and $c_2 = 0$, we have $\langle x\rangle = a/\sqrt{2}$.

(d) In the special case where $c_0 = 1/\sqrt{2}$, $c_1 = \mathrm{i}/\sqrt{2}$ and $c_2 = 0$, we have $\langle x\rangle = 0$.

Answer D2

(a) Using the coefficient rule, we have

$$1 = |A/2|^2 + |A|^2 = \tfrac{5}{4}|A|^2,$$

so $|A|^2 = 4/5$. If A is real and positive, we have $A = \sqrt{4/5}$. The other possible values are $(4/5)\mathrm{e}^{\mathrm{i}\phi}$ where ϕ is real. A multiplicative phase factor $\mathrm{e}^{\mathrm{i}\phi}$ makes no difference to the state, so all these values correspond to the same state.

(b) Using the coefficient rule, we have

$$1 = |1/2|^2 + |\alpha|^2,$$

so $|\alpha|^2 = 3/4$. If α is real and positive, we have $\alpha = \sqrt{3}/2$. The other possible values are $(\sqrt{3}/2)\mathrm{e}^{\mathrm{i}\phi}$ where ϕ is real. Here, α is NOT a factor multiplying the whole wave function. In this case, the state is in general changed by changing the phase of α.

Answer D3

Remembering that $\psi_1(x)$ and $\psi_2(x)$ are real, the probability density is

$$\Psi^*(x,t)\,\Psi(x,t) = \frac{1}{2}\left(\psi_1\exp[\mathrm{i}E_1t/\hbar] + \psi_2\exp[\mathrm{i}E_2t/\hbar]\right)\left(\psi_1\exp[-\mathrm{i}E_1t/\hbar] + \psi_2\exp[-\mathrm{i}E_2t/\hbar]\right)$$
$$= \frac{1}{2}(\psi_1^2 + \psi_2^2) + \frac{1}{2}\psi_1\psi_2\left(\exp[\mathrm{i}(E_2 - E_1)t/\hbar] + \exp[-\mathrm{i}(E_2 - E_1)t/\hbar]\right)$$
$$= \frac{1}{2}(\psi_1^2 + \psi_2^2) + \psi_1\psi_2\cos[(E_2 - E_1)t/\hbar].$$

So the probability density varies sinusoidally with time with angular frequency $\omega = |E_2 - E_1|/\hbar$ and period

$$T = \frac{2\pi}{\omega} = \frac{2\pi\hbar}{|E_2 - E_1|} = \frac{h}{|E_2 - E_1|}.$$

Answer D4

(a) The normalization condition is

$$\sum_n |a_n|^2 = 1,$$

so

$$|A|^2 + 4|A|^2 + |A|^2 = 6|A|^2 = 1.$$

Hence $|A|^2 = 1/6$. Choosing A to be real and positive, the normalization constant is $A = 1/\sqrt{6}$.

(b) The probability of finding $E_1 = 3\hbar\omega_0/2$ is $|a_1|^2 = 4|A|^2 = 2/3$.

(c) The probability of finding $E_2 = 5\hbar\omega_0/2$ is $|a_2|^2 = 0$.

(d) The probability of finding a value greater than $\hbar\omega_0$ is

$$|a_1|^2 + |a_2|^2 + |a_3|^2 + \ldots = 4|A|^2 + |A|^2 = 5/6.$$

This could also be calculated as $1 - |a_0|^2$, because it is the probability of NOT getting the ground-state energy, $\hbar\omega_0/2$.

(e) The expectation value of the energy is

$$\begin{aligned}\langle E\rangle &= \sum_n E_n|a_n|^2 \\ &= \tfrac{1}{6}E_0 + \tfrac{4}{6}E_1 + \tfrac{1}{6}E_3 = \left(\tfrac{1}{6}\cdot\tfrac{1}{2} + \tfrac{4}{6}\cdot\tfrac{3}{2} + \tfrac{1}{6}\cdot\tfrac{7}{2}\right)\hbar\omega_0 = \tfrac{5}{3}\hbar\omega_0.\end{aligned}$$

(f) The measurement causes the wave function to collapse, so after the measurement, the state is $\psi_1(x)\exp(-\mathrm{i}E_1t/\hbar) = \psi_1(x)\exp(-\mathrm{i}3\omega_0t/2)$. (The factor $\exp(-\mathrm{i}3\omega_0t/2)$ could be omitted because overall multiplicative phase factors like this do not affect the state being described.) The collapsed state is a stationary state, and any subsequent measurement of the energy is certain to give the corresponding eigenvalue, $E_1 = 3\hbar\omega_0/2$.

Answer D5

The wave packet is normalized, so the coefficient rule gives the following probabilities for energy values E_0, E_1 and E_3:

$$p_0 = \frac{1}{6}, \quad p_1 = \frac{4}{6}, \quad p_3 = \frac{1}{6}.$$

Hence the expectation value of the energy is

$$\langle E\rangle = p_0E_0 + p_1E_1 + p_3E_3 = \tfrac{1}{6}\cdot\tfrac{1}{2}\hbar\omega_0 + \tfrac{4}{6}\cdot\tfrac{3}{2}\hbar\omega_0 + \tfrac{1}{6}\cdot\tfrac{7}{2}\hbar\omega_0 = \tfrac{20}{12}\hbar\omega_0 = \tfrac{5}{3}\hbar\omega_0.$$

The expectation value of E^2 is

$$\langle E^2\rangle = \left(\tfrac{1}{6}\cdot\tfrac{1}{4} + \tfrac{4}{6}\cdot\tfrac{9}{4} + \tfrac{1}{6}\cdot\tfrac{49}{4}\right)\hbar^2\omega_0^2 = \tfrac{43}{12}\hbar^2\omega_0^2.$$

So the uncertainty in the energy is given by

$$(\Delta E)^2 = \langle E^2\rangle - \langle E\rangle^2 = \left(\tfrac{43}{12} - \tfrac{25}{9}\right)\hbar^2\omega_0^2 = \tfrac{29}{36}\,\hbar^2\omega_0^2.$$

Therefore

$$\Delta E = \sqrt{\frac{29}{36}}\hbar\omega_0 \approx 0.898\,\hbar\omega_0.$$

Answer D6

(a) The normalization condition is $\sum_n |a_n|^2 = 1$, so

$$|N|^2(4+1) = 1.$$

Hence $|N|^2 = 1/5$. Taking N to be real and positive, we get $N = 1/\sqrt{5}$.

(b) Using the coefficient rule, the probabilities of getting energies $E_0 = \hbar\omega_0/2$ and $E_1 = 3\hbar\omega_0/2$ are

$$p_0 = \frac{4}{5} \quad \text{and} \quad p_1 = \frac{1}{5}.$$

So the expectation value of E is

$$\langle E\rangle = p_0E_0 + p_1E_1 = \tfrac{4}{5}\cdot\tfrac{1}{2}\hbar\omega_0 + \tfrac{1}{5}\cdot\tfrac{3}{2}\hbar\omega_0 = \tfrac{7}{10}\hbar\omega_0.$$

The expectation value of E^2 is

$$\langle E^2\rangle = p_0E_0^2 + p_1E_1^2 = \left(\tfrac{4}{5}\cdot\left(\tfrac{1}{2}\right)^2 + \tfrac{1}{5}\cdot\left(\tfrac{3}{2}\right)^2\right)\hbar^2\omega_0^2 = \tfrac{13}{20}\hbar^2\omega_0^2.$$

Thus

$$\Delta E = [\langle E^2\rangle - \langle E\rangle^2]^{1/2} = \left[\tfrac{13}{20} - \left(\tfrac{7}{10}\right)^2\right]^{1/2}\hbar\omega_0 = \tfrac{2}{5}\hbar\omega_0.$$

(c) At any time $t_1 > 0$, the wave function is

$$\begin{aligned}\Psi(x,t_1) &= \frac{1}{\sqrt{5}}\left(2\psi_0(x)\,\mathrm{e}^{-\mathrm{i}E_0t_1/\hbar} + \psi_1(x)\,\mathrm{e}^{-\mathrm{i}E_1t_1/\hbar}\right)\\ &= \frac{1}{\sqrt{5}}\left(2\psi_0(x)\,\mathrm{e}^{-\mathrm{i}\omega_0t_1/2} + \psi_1(x)\,\mathrm{e}^{-\mathrm{i}3\omega_0t_1/2}\right)\end{aligned}$$

The probabilities of getting values E_0 and E_1 at a time $t_1 > 0$ are then

$$p_0 = \left|\frac{2}{\sqrt{5}}\mathrm{e}^{-\mathrm{i}\omega_0t_1/2}\right|^2 = \frac{4}{5}$$

$$p_1 = \left|\frac{1}{\sqrt{5}}\mathrm{e}^{-\mathrm{i}3\omega_0t_1/2}\right|^2 = \frac{1}{5},$$

which are the same as the probabilities at $t = 0$. (It follows that $\langle E\rangle$ and ΔE are also unchanged.) The probability of finding $E_0 = \frac{1}{2}\hbar\omega_0$ is $|a_0|^2 = 4/5$.

(d) A second measurement of energy on the same system is certain to yield the same value, as the wave function collapses to an eigenstate at the first measurement. So the probability is equal to 1.

Answer D7

(a) The momentum amplitude is given by

$$\begin{aligned}A(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x\\ &= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{a\sqrt{\pi}}\right)^{1/2}\int_{-\infty}^{\infty}\mathrm{e}^{-x^2/2a^2}\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x\end{aligned}$$

Using the given standard integral, we get

$$\begin{aligned}A(k) &= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{a\sqrt{\pi}}\right)^{1/2}\sqrt{2\pi}a\,\mathrm{e}^{-a^2k^2/2}\\ &= \left(\frac{a}{\sqrt{\pi}}\right)^{1/2}\mathrm{e}^{-a^2k^2/2}.\end{aligned}$$

(b) The small momentum range between $-0.01\hbar/a$ and $+0.01\hbar/a$ is centred on $\hbar k = 0$, and has width $\delta k = 0.02\hbar/a$. So the probability of getting a momentum in this range is

$$\text{probability} = |A(0)|^2\,\delta k = \frac{a}{\sqrt{\pi}}\cdot\frac{0.02}{a} = \frac{0.02}{\sqrt{\pi}} \simeq 0.001\,13.$$

(c) At any time $t > 0$, the wave function is

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)\exp(\mathrm{i}kx - \hbar k^2t/2m)\,\mathrm{d}k\\ &= \left(\frac{a}{2\pi^{3/2}}\right)^{1/2}\int_{-\infty}^{\infty}\exp(\mathrm{i}kx - k^2(a^2 + \hbar t/m)/2)\,\mathrm{d}k.\end{aligned}$$

E: Orbital angular momentum

Answer E1

Using $\widehat{L}_z = -i\hbar(x\partial/\partial y - y\partial/\partial x)$ in Cartesian coordinates, and $\widehat{L}_z = -i\hbar\partial/\partial\phi$ in plane polars, with $x = r\cos\phi$ and $y = r\sin\phi$, we have:

(i)	$\widehat{L}_z(x) = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)x = i\hbar y$	no
(ii)	$\widehat{L}_z(xy) = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)xy = i\hbar(x^2 - y^2)$	no
(iii)	$\widehat{L}_z(x^2 + y^2) = \widehat{L}_z r^2 = -i\hbar\frac{\partial}{\partial\phi}r^2 = 0$	yes, eigenvalue 0
(iv)	$\widehat{L}_z(x + iy) = \widehat{L}_z(r\cos\phi + i\sin\phi) = -i\hbar\frac{\partial}{\partial\phi}(re^{i\phi}) = \hbar re^{i\phi}$	yes, eigenvalue $\hbar$
(v)	$\widehat{L}_z(x - iy)^2 = -i\hbar\frac{\partial}{\partial\phi}(r^2e^{-2i\phi}) = -2\hbar r^2e^{-2i\phi}$	yes, eigenvalue $-2\hbar$
(vi)	$\widehat{L}_z(r^2\sin\phi) = -i\hbar\frac{\partial}{\partial\phi}(r^2\sin\phi) = -i\hbar r^2\cos\phi$	no
(vii)	$\widehat{L}_z(re^{i\phi}) = -i\hbar\frac{\partial}{\partial\phi}(re^{i\phi}) = \hbar re^{i\phi}$	yes, eigenvalue $\hbar$
(viii)	$\widehat{L}_z(e^{i\phi} + e^{-i\phi}) = -i\hbar\frac{\partial}{\partial\phi}(e^{i\phi} + e^{-i\phi}) = \hbar(e^{i\phi} - e^{-i\phi})$	no

Answer E2

(a) In plane polar coordinates

$$\widehat{L}_z = -i\hbar\frac{\partial}{\partial\phi}.$$

The eigenvalue equation,

$$-i\hbar\frac{\partial}{\partial\phi}\,\psi(r,\phi) = L_z\psi(r,\phi),$$

has solution

$$\psi(r,\phi) = AR(r)\,\exp\left(i\frac{L_z}{\hbar}\phi\right),$$

for any function $R(r)$. The boundary condition

$$\psi(r,\phi + 2\pi) = \psi(r,\phi)$$

gives

$$\exp(i2\pi L_z/\hbar) = 1,$$

that is

$$2\pi L_z/\hbar = 2\pi m \qquad (m = 0, \pm1, \pm2, \ldots).$$

So

$$L_z = m\hbar,$$

where m is an integer, positive, negative or zero.

The eigenfunctions are thus

$$\psi_m(r,\phi) = R(r)\exp(im\phi),$$

where m is an integer and $R(r)$ is any function of r. The corresponding eigenvalues are

$$L_z = m\hbar.$$

(b) The orthogonality integral is

$$\int_{\phi=0}^{\phi=2\pi}\int_{r=0}^{r=\infty}\psi_m^*(r,\phi)\,\psi_n(r,\phi)\,r\,dr\,d\phi = \int_{r=0}^{r=\infty}R_m^*(r)\,R_n(r)\,dr\int_{\phi=0}^{\phi=2\pi}\exp(i(n-m)\phi)\,d\phi.$$

The second integral is

$$\int_0^{2\pi} \exp(\mathrm{i}(n-m)\phi)\,\mathrm{d}\phi = \left[\frac{1}{\mathrm{i}(n-m)}\exp(\mathrm{i}(n-m)\phi)\right]_0^{2\pi} = 0$$

for $m \neq n$. Hence $\psi_m(r,\phi)$ is orthogonal to $\psi_n(r,\phi)$ for $m \neq n$.

(c) The normalization condition is

$$\int_{\phi=0}^{\phi=2\pi}\int_{r=0}^{r=\infty} |\psi(r,\phi)|^2 r\,\mathrm{d}r\,\mathrm{d}\phi = 1.$$

Using the integrals given in the question we have

$$1 = |A|^2 \int_{\phi=0}^{\phi=2\pi} \sin^2(3\phi)\,\mathrm{d}\phi \int_{r=0}^{r=\infty} r|R(r)|^2\,\mathrm{d}r = |A|^2\pi,$$

so an acceptable solution is

$$A = \frac{1}{\sqrt{\pi}}.$$

(d) Using the sandwich rule,

$$\begin{aligned}
\langle L_z\rangle &= \int \psi^* \widehat{\mathrm{L}}_z \psi\,\mathrm{d}V \\
&= \frac{1}{\pi}\int_{\phi=0}^{\phi=2\pi}\int_{r=0}^{r=\infty} (R^*(r)\sin(3\phi))\left(-\mathrm{i}\hbar\frac{\partial}{\partial\phi}\right)(R(r)\sin(3\phi))\,r\,\mathrm{d}r\,\mathrm{d}\phi \\
&= -\frac{\mathrm{i}\hbar}{\pi}\int_{r=0}^{r=\infty} r|R(r)|^2\,\mathrm{d}r \int_{\phi=0}^{\phi=2\pi} 3\sin(3\phi)\,\cos(3\phi)\,\mathrm{d}\phi \\
&= -\frac{3\mathrm{i}\hbar}{2\pi}\int_0^{2\pi}\sin(6\phi)\,\mathrm{d}\phi \\
&= \frac{\mathrm{i}\hbar}{4\pi}\left[\cos(6\phi)\right]_{\phi=0}^{\phi=2\pi} \\
&= 0.
\end{aligned}$$

(e) Using Euler's formula,

$$\psi(r,\phi) = \frac{1}{\sqrt{\pi}}R(r)\sin(3\phi) = \frac{1}{2\mathrm{i}}\frac{1}{\sqrt{\pi}}R(r)\,\left(\exp(3\mathrm{i}\phi) - \exp(-3\mathrm{i}\phi)\right).$$

(f) Since ψ is an equal mixture of two eigenfunctions of $\widehat{\mathrm{L}}_z$, the probabilities of obtaining $L_z = 3\hbar$ and $L_z = -3\hbar$ are both $\frac{1}{2}$.

(g) Using the result of part (f),

$$\langle L_z\rangle = \frac{1}{2}(3\hbar) + \frac{1}{2}(-3\hbar) = 0,$$

which agrees with the answer to part (d).

Answer E3

(a) The variable ϕ appears in $\widehat{\mathrm{L}}^2$ only as $\frac{\partial^2}{\partial\phi^2}$. Since $\frac{\partial}{\partial\phi}$ and $\frac{\partial^2}{\partial\phi^2}$ commute with one another, it follows that $\widehat{\mathrm{L}}_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}$ commutes with $\widehat{\mathrm{L}}^2$. This means that it is possible to find a set of functions which are simultaneous eigenfunctions of $\widehat{\mathrm{L}}_z$ and $\widehat{\mathrm{L}}^2$.

(b)

$$\begin{aligned}
\widehat{\mathrm{L}}_z Y_{l,m} &= -\mathrm{i}\hbar\frac{\partial}{\partial\phi}\,(A\sin(2\theta)\,\exp(\mathrm{i}\phi)) \\
&= (-\mathrm{i}\hbar)\,(\mathrm{i})\,(A\sin(2\theta)\,\exp(\mathrm{i}\phi)) \\
&= \hbar Y_{l,m}.
\end{aligned}$$

Also

$$\widehat{\mathrm{L}}^2 Y_{l,m} = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) (A \sin(2\theta)\, \exp(\mathrm{i}\phi))$$

$$= (-\hbar^2)\,(A) \left(-4\sin(2\theta) + 2\cot\theta\cos(2\theta) - \frac{\sin(2\theta)}{\sin^2\theta} \right) \exp(\mathrm{i}\phi)$$

$$= -\hbar^2 A \left(-4\sin(2\theta) + 2\frac{\cos\theta}{\sin\theta}\,(1 - 2\sin^2\theta) - \frac{2\sin\theta\cos\theta}{\sin^2\theta} \right) \exp(\mathrm{i}\phi)$$

$$= -\hbar^2 A(-4\sin(2\theta) - 4\cos\theta\sin\theta)\exp(\mathrm{i}\phi)$$

$$= 6\hbar^2 A\sin(2\theta)\, \exp(\mathrm{i}\phi) = 6\hbar^2\, Y_{l,m}.$$

So $Y_{l,m}(\theta,\phi)$ is an eigenfunction of $\widehat{\mathrm{L}}_z$ with eigenvalue $\hbar$, corresponding to $m = 1$, and an eigenfunction of $\widehat{\mathrm{L}}^2$ with eigenvalue $6\hbar^2$, corresponding to $l = 2$.

(c) The normalization condition is

$$1 = \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} |Y_{l,m}|^2 \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi.$$

So

$$1 = |A|^2 \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \sin^2(2\theta)\, \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$$

$$= |A|^2 \int_{\phi=0}^{\phi=\pi} \int_{\theta=0}^{\theta=\pi} 4\sin^3\theta\cos^2\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$$

$$= 8\pi\, |A|^2 \int_{\theta=0}^{\theta=\pi} \sin^3\theta\cos^2\theta\, \mathrm{d}\theta$$

$$= (8\pi)\frac{4}{15}|A|^2$$

$$= \frac{32}{15}\,\pi|A|^2.$$

Choosing the normalization constant A to be real and positive,

$$A = \sqrt{\frac{15}{32\pi}}.$$

Answer E4

(a) Expanding the commutators on the right-hand side gives

$$\widehat{\mathrm{A}}\left[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\right] + \left[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\right]\widehat{\mathrm{A}} = \widehat{\mathrm{A}}\widehat{\mathrm{A}}\widehat{\mathrm{B}} - \widehat{\mathrm{A}}\widehat{\mathrm{B}}\widehat{\mathrm{A}} + \widehat{\mathrm{A}}\widehat{\mathrm{B}}\widehat{\mathrm{A}} - \widehat{\mathrm{B}}\widehat{\mathrm{A}}\widehat{\mathrm{A}}$$

$$= \widehat{\mathrm{A}}\widehat{\mathrm{A}}\widehat{\mathrm{B}} - \widehat{\mathrm{B}}\widehat{\mathrm{A}}\widehat{\mathrm{A}}$$

$$= \left[\widehat{\mathrm{A}}^2, \widehat{\mathrm{B}}\right].$$

(b) Using the identity that we found in part (a), and the commutation relations given in the question, we have

$$\left[\widehat{\mathrm{L}}_x^2, \widehat{\mathrm{L}}_z\right] = \widehat{\mathrm{L}}_x\left[\widehat{\mathrm{L}}_x, \widehat{\mathrm{L}}_z\right] + \left[\widehat{\mathrm{L}}_x, \widehat{\mathrm{L}}_z\right]\widehat{\mathrm{L}}_x$$

$$= -\mathrm{i}\hbar\left(\widehat{\mathrm{L}}_x\widehat{\mathrm{L}}_y + \widehat{\mathrm{L}}_y\widehat{\mathrm{L}}_x\right)$$

and

$$\left[\widehat{\mathrm{L}}_y^2, \widehat{\mathrm{L}}_z\right] = \widehat{\mathrm{L}}_y\left[\widehat{\mathrm{L}}_y, \widehat{\mathrm{L}}_z\right] + \left[\widehat{\mathrm{L}}_y, \widehat{\mathrm{L}}_z\right]\widehat{\mathrm{L}}_y$$

$$= +\mathrm{i}\hbar\left(\widehat{\mathrm{L}}_y\widehat{\mathrm{L}}_x + \widehat{\mathrm{L}}_x\widehat{\mathrm{L}}_y\right).$$

Also,

$$\left[\widehat{\mathrm{L}}_z^2, \widehat{\mathrm{L}}_z\right] = \widehat{\mathrm{L}}_z\widehat{\mathrm{L}}_z\widehat{\mathrm{L}}_z - \widehat{\mathrm{L}}_z\widehat{\mathrm{L}}_z\widehat{\mathrm{L}}_z = 0.$$

We have $\widehat{\mathrm{L}}^2 = \widehat{\mathrm{L}}_x^2 + \widehat{\mathrm{L}}_y^2 + \widehat{\mathrm{L}}_z^2$, so

$$\begin{aligned}\left[\widehat{\mathrm{L}}^2, \widehat{\mathrm{L}}_z\right] &= \left[\widehat{\mathrm{L}}_x^2, \widehat{\mathrm{L}}_z\right] + \left[\widehat{\mathrm{L}}_y^2, \widehat{\mathrm{L}}_z\right] + \left[\widehat{\mathrm{L}}_z^2, \widehat{\mathrm{L}}_z\right] \\ &= -\mathrm{i}\hbar\left(\widehat{\mathrm{L}}_x\widehat{\mathrm{L}}_y + \widehat{\mathrm{L}}_y\widehat{\mathrm{L}}_x\right) + \mathrm{i}\hbar\left(\widehat{\mathrm{L}}_x\widehat{\mathrm{L}}_y + \widehat{\mathrm{L}}_y\widehat{\mathrm{L}}_x\right) + 0 \\ &= 0,\end{aligned}$$

as required.

(c) In general, it is not possible to find simultaneous eigenfunctions of the operators $\widehat{\mathrm{L}}_x$, $\widehat{\mathrm{L}}_y$ and $\widehat{\mathrm{L}}_z$.

(d) It is possible to find a set of states which are simultaneously eigenfunctions of $\widehat{\mathrm{L}}^2$ and of any one of the components of angular momentum.

(e) The operator is

$$\widehat{\mathrm{L}}_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}.$$

Its eigenfunctions are

$$\psi(r,\,\theta,\,\phi) = A\,f(r,\theta)\exp(\mathrm{i}m\phi)$$

with corresponding eigenvalues $m\hbar$, where m is an integer, positive, negative or zero.

(f) The eigenvalues of $\widehat{\mathrm{L}}^2$ are $l(l+1)\hbar^2$, with $l = 0,\,1,\,2,\,3,\ldots$. For each value of l, there are $(2l+1)$ different (technically, linearly independent) eigenfunctions, corresponding to $m = -l,\,-l+1,\ldots-1,\,0,\,1,\ldots,l-1,\,l$.

(g)

$$\begin{aligned}\widehat{\mathrm{L}}^2\psi(\theta,\phi) &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\psi(\theta,\phi) \\ &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)(A\sin\theta\cos\phi) \\ &= -\hbar^2 A\left(-\sin\theta\cos\phi + \cot\theta\cos\theta\cos\phi - \frac{1}{\sin^2\theta}\sin\theta\cos\phi\right) \\ &= -\hbar^2 A\left(-\sin\theta\cos\phi + \frac{\cos^2\theta}{\sin\theta}\cos\phi - \frac{1}{\sin\theta}\cos\phi\right) \\ &= -\hbar^2 A\left(-\sin\theta\cos\phi - \frac{(1-\cos^2\theta)}{\sin\theta}\cos\phi\right) \\ &= -\hbar^2 A\left(-\sin\theta\cos\phi - \frac{\sin^2\theta}{\sin\theta}\cos\phi\right) \\ &= 2\hbar^2 A\sin\theta\cos\phi = 2\hbar^2\psi(\theta,\,\phi).\end{aligned}$$

So $\psi(\theta,\phi)$ is an eigenfunction of $\widehat{\mathrm{L}}^2$ with eigenvalue $2\hbar^2$, which corresponds to $l = 1$.

$$\begin{aligned}\widehat{\mathrm{L}}_z\psi(\theta,\phi) &= -\mathrm{i}\hbar\frac{\partial}{\partial\phi}(A\sin\theta\cos\phi) \\ &= \mathrm{i}\hbar A\sin\theta\sin\phi.\end{aligned}$$

So $\psi(\theta,\phi)$ is not an eigenfunction of $\widehat{\mathrm{L}}_z$.

(h) There are $(2l+1)$ different (technically, linearly independent) functions with the same value of L^2 but different values of L_z. Any linear combination of these functions will also be an eigenfunction of $\widehat{\mathrm{L}}^2$, but will not in general, be an eigenfunction of $\widehat{\mathrm{L}}_z$. So there is no contradiction.

(i)

$$\psi(r,\theta,\,\phi) = R(r)\,\sin\theta\,\cos\phi = \frac{1}{2}R(r)\,\sin\theta\,(\exp(\mathrm{i}\phi)+\exp(-\mathrm{i}\phi)).$$

So ψ is a linear combination of two eigenfunctions of $\widehat{\mathrm{L}}_z$ with eigenvalues $+\hbar$ and $-\hbar$. These two outcomes have equal probabilities, namely $\frac{1}{2}$.

(j) A measurement of $\widehat{\mathrm{L}}^2$ is certain to give an outcome of $2\hbar^2$, whereas a measurement of $\widehat{\mathrm{L}}_z$ has possible outcomes of $+\hbar$ and $-\hbar$ with equal probabilities.

F: Spin angular momentum

Answer F1

(a) The probability amplitude for measuring $S_y = -\frac{1}{2}\hbar$ is

$$\langle\downarrow_y|A\rangle = \frac{1}{\sqrt{5}}\frac{1}{\sqrt{2}}\begin{bmatrix}-\mathrm{i} & 1\end{bmatrix}\begin{bmatrix}1\\2\mathrm{i}\end{bmatrix} = \frac{1}{\sqrt{10}}(-\mathrm{i}+2\mathrm{i}) = \frac{\mathrm{i}}{\sqrt{10}}.$$

So the probability of measuring $S_y = -\frac{1}{2}\hbar$ is

$$|\langle\downarrow_y|A\rangle|^2 = \frac{1}{10}.$$

(We can also conclude that the probability of measuring $S_y = +\frac{1}{2}\hbar$ is $1-\frac{1}{10}=\frac{9}{10}$.)

(b) The expectation value $\langle S_y\rangle$ is

$$\begin{aligned}\langle A|\widehat{\mathrm{S}}_y|A\rangle &= \frac{1}{\sqrt{5}}\frac{1}{\sqrt{5}}\frac{\hbar}{2}\begin{bmatrix}1 & -2\mathrm{i}\end{bmatrix}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\begin{bmatrix}1\\2\mathrm{i}\end{bmatrix} = \frac{1}{10}\hbar\begin{bmatrix}1 & -2\mathrm{i}\end{bmatrix}\begin{bmatrix}2\\ \mathrm{i}\end{bmatrix}\\ &= \frac{1}{10}\hbar(2+2) = \frac{2}{5}\hbar.\end{aligned}$$

We also have

$$\widehat{\mathrm{S}}_y^2 = \frac{\hbar^2}{4}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix} = \frac{\hbar^2}{4}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}.$$

So

$$\langle A|\widehat{\mathrm{S}}_y^2|A\rangle = \frac{\hbar^2}{4}\langle A|A\rangle = \frac{\hbar^2}{4}.$$

Alternatively we can use the result of part (a):

$$\langle S_y\rangle = \left(\frac{9}{10}\right)\left(\frac{1}{2}\hbar\right)+\left(\frac{1}{10}\right)\left(-\frac{1}{2}\hbar\right) = \frac{2}{5}\hbar.$$

For S_y^2, the possible values are $(\pm\hbar/2)^2 = \hbar^2/4$. Hence

$$\langle S_y^2\rangle = \left(\frac{9}{10}\right)\left(\frac{\hbar^2}{4}\right)+\left(\frac{1}{10}\right)\left(\frac{\hbar^2}{4}\right) = \frac{\hbar^2}{4}.$$

(c) The uncertainty in the value of S_y is

$$\Delta S_y = (\langle S_y^2\rangle - \langle S_y\rangle^2)^{1/2} = \left(\frac{\hbar^2}{4}-\left(\frac{2}{5}\hbar\right)^2\right)^{1/2} = \left(\frac{1}{4}-\frac{4}{25}\right)^{1/2}\hbar = \frac{3}{10}\hbar.$$

(d) After the measurement of $S_z = -\frac{1}{2}\hbar$, the state will collapse to $|\downarrow_z\rangle$. We need to express this is as linear combination of $|\uparrow_y\rangle$ and $|\downarrow_y\rangle$. So, let

$$|\downarrow_z\rangle = a|\uparrow_y\rangle + b|\downarrow_y\rangle,$$

where a and b are constants. Then

$$a = \langle\uparrow_y|\downarrow_z\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & -\mathrm{i}\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = -\frac{\mathrm{i}}{\sqrt{2}}$$

$$b = \langle\downarrow_y \mid \downarrow_z\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}-\mathrm{i} & 1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}.$$

So the state immediately after the measurement can be expressed as

$$-\frac{\mathrm{i}}{\sqrt{2}}\mid\uparrow_y\rangle + \frac{1}{\sqrt{2}}\mid\downarrow_y\rangle.$$

The probability of measuring $S_y = -\hbar/2$ is then $1/2$.

Answer F2

(a)

$$\widehat{\mathrm{S}}_x|A\rangle_{\text{initial}} = \frac{\hbar}{2\sqrt{2}}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}1\\1\end{bmatrix} = \frac{\hbar}{2\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} = \frac{1}{2}\hbar\,|A\rangle_{\text{initial}}.$$

So $|A\rangle_{\text{initial}}$ is an eigenvector of $\widehat{\mathrm{S}}_x$ with eigenvalue $\frac{1}{2}\hbar$, as required.

(b) We have

$$\widehat{\mathrm{H}}\mid\uparrow_z\rangle = \frac{\hbar\omega}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \frac{\hbar\omega}{2}\begin{bmatrix}1\\0\end{bmatrix} = \frac{\hbar\omega}{2}\mid\uparrow_z\rangle$$

and

$$\widehat{\mathrm{H}}\mid\downarrow_z\rangle = \frac{\hbar\omega}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = -\frac{\hbar\omega}{2}\begin{bmatrix}0\\1\end{bmatrix} = -\frac{\hbar\omega}{2}\mid\downarrow_z\rangle.$$

So $\mid\uparrow_z\rangle$ and $\mid\downarrow_z\rangle$ are eigenvectors of $\widehat{\mathrm{H}} = \omega\widehat{\mathrm{S}}_z$ with eigenvalues $E_{\mathrm{u}} = \frac{1}{2}\hbar\omega$ and $E_{\mathrm{d}} = -\frac{1}{2}\hbar\omega$.

(c) By inspection

$$|A\rangle_{\text{initial}} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\end{bmatrix} + \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\mid\uparrow_z\rangle + \frac{1}{\sqrt{2}}\mid\downarrow_z\rangle.$$

So the time evolution of the state is

$$\begin{aligned}|A\rangle &= \frac{1}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}E_{\mathrm{u}}t/\hbar}\mid\uparrow_z\rangle + \frac{1}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}E_{\mathrm{d}}t/\hbar}\mid\downarrow_z\rangle\\ &= \frac{1}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}\omega t/2}\mid\uparrow_z\rangle + \frac{1}{\sqrt{2}}\,\mathrm{e}^{\mathrm{i}\omega t/2}\mid\downarrow_z\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}\mathrm{e}^{-\mathrm{i}\omega t/2}\\ \mathrm{e}^{\mathrm{i}\omega t/2}\end{bmatrix}.\end{aligned}$$

(d) The probability amplitude of a measurement of $S_x = -\frac{1}{2}\hbar$ is

$$\langle\downarrow_x|A\rangle = \frac{1}{2}\begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}\mathrm{e}^{-\mathrm{i}\omega t/2}\\ \mathrm{e}^{\mathrm{i}\omega t/2}\end{bmatrix} = \frac{1}{2}\left(\mathrm{e}^{\mathrm{i}\omega t/2} + \mathrm{e}^{-\mathrm{i}\omega t/2}\right) = \cos\left(\tfrac{1}{2}\omega t\right).$$

So the probability of a measurement of $S_x = -\frac{1}{2}\hbar$ is

$$|\langle\downarrow_x|A\rangle|^2 = \cos^2\left(\tfrac{1}{2}\omega t\right).$$

Answer F3

(a)

$$\langle\uparrow_y \mid \uparrow_y\rangle = \frac{1}{2}\begin{bmatrix}1 & -\mathrm{i}\end{bmatrix}\begin{bmatrix}1\\ \mathrm{i}\end{bmatrix} = \frac{1}{2}(1+1) = 1.$$

$$\langle\downarrow_y \mid \downarrow_y\rangle = \frac{1}{2}\begin{bmatrix}-\mathrm{i} & 1\end{bmatrix}\begin{bmatrix}\mathrm{i}\\1\end{bmatrix} = \frac{1}{2}(1+1) = 1.$$

$$\langle\uparrow_y \mid \downarrow_y\rangle = \frac{1}{2}\begin{bmatrix}1 & -\mathrm{i}\end{bmatrix}\begin{bmatrix}\mathrm{i}\\1\end{bmatrix} = \frac{1}{2}(\mathrm{i}-\mathrm{i}) = 0.$$

So $|\uparrow_y\rangle$ and $|\downarrow_y\rangle$ are orthonormal.

(b) We have

$$\widehat{\mathrm{H}}|\uparrow_y\rangle = \frac{\hbar\omega}{2\sqrt{2}}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\begin{bmatrix}1\\ \mathrm{i}\end{bmatrix} = \frac{\hbar\omega}{2\sqrt{2}}\begin{bmatrix}1\\ \mathrm{i}\end{bmatrix} = \frac{\hbar\omega}{2}|\uparrow_y\rangle$$

and

$$\widehat{\mathrm{H}}|\downarrow_y\rangle = \frac{\hbar\omega}{2\sqrt{2}}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\begin{bmatrix}\mathrm{i}\\ 1\end{bmatrix} = -\frac{\hbar\omega}{2\sqrt{2}}\begin{bmatrix}\mathrm{i}\\ 1\end{bmatrix} = -\frac{\hbar\omega}{2}|\downarrow_y\rangle.$$

So $|\uparrow_y\rangle$ and $|\downarrow_y\rangle$ are eigenvectors of $\widehat{\mathrm{H}} = \omega\widehat{\mathrm{S}}_y$ with eigenvalues $E_{\mathrm{u}} = \frac{1}{2}\hbar\omega$ and $E_{\mathrm{d}} = -\frac{1}{2}\hbar\omega$.

(c) Putting $t = 0$ in the expression for $|A\rangle$,

$$|A\rangle_{\text{initial}} = a_{\mathrm{u}}|\uparrow_y\rangle + a_{\mathrm{d}}|\downarrow_y\rangle.$$

So

$$a_{\mathrm{u}} = \langle\uparrow_y|A\rangle_{\text{initial}} = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & -\mathrm{i}\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix} = \frac{1}{\sqrt{2}},$$

$$a_{\mathrm{d}} = \langle\downarrow_y|A\rangle_{\text{initial}} = \frac{1}{\sqrt{2}}\begin{bmatrix}-\mathrm{i} & 1\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix} = -\frac{\mathrm{i}}{\sqrt{2}}.$$

(d)

$$\begin{aligned}
|A\rangle &= a_{\mathrm{u}}\exp(-\mathrm{i}E_{\mathrm{u}}t/h)|\uparrow_y\rangle + a_{\mathrm{d}}\exp(-\mathrm{i}E_{\mathrm{d}}t/\hbar)|\downarrow_y\rangle\\
&= \frac{1}{2}\,\mathrm{e}^{-\mathrm{i}\omega t/2}\begin{bmatrix}1\\ \mathrm{i}\end{bmatrix} + \frac{-\mathrm{i}}{2}\,\mathrm{e}^{\mathrm{i}\omega t/2}\begin{bmatrix}\mathrm{i}\\ 1\end{bmatrix}\\
&= \frac{1}{2}\begin{bmatrix}\mathrm{e}^{-\mathrm{i}\omega t/2} + \mathrm{e}^{\mathrm{i}\omega t/2}\\ \mathrm{i}\mathrm{e}^{-\mathrm{i}\omega t/2} - \mathrm{i}\mathrm{e}^{\mathrm{i}\omega t/2}\end{bmatrix} = \begin{bmatrix}\cos(\omega t/2)\\ \sin(\omega t/2)\end{bmatrix}\\
&= \cos(\omega t/2)|\uparrow_z\rangle + \sin(\omega t/2)|\downarrow_z\rangle.
\end{aligned}$$

So the probability of a measurement $S_z = \frac{1}{2}\hbar$ is $\cos^2(\frac{1}{2}\omega t)$. Similarly the probability of a measurement of $S_z = -\frac{1}{2}\hbar$ is $\sin^2(\frac{1}{2}\omega t)$. (Alternatively, we could have evaluated $|\langle\uparrow_z|A\rangle|^2$ and $|\langle\downarrow_z|A\rangle|^2$.)

(e) The expectation value $\langle S_z\rangle$ is

$$\begin{aligned}
\langle S_z\rangle &= \left(\cos^2(\tfrac{1}{2}\omega t)\right)\left(\tfrac{1}{2}\hbar\right) + \left(\sin^2(\tfrac{1}{2}\omega t)\right)\left(-\tfrac{1}{2}\hbar\right)\\
&= \frac{1}{2}\hbar\left(\cos^2(\tfrac{1}{2}\omega t) - \sin^2(\tfrac{1}{2}\omega t)\right)\\
&= \frac{1}{2}\hbar\cos(\omega t).
\end{aligned}$$

Alternatively we could have used the formula

$$\begin{aligned}
\langle S_z\rangle &= \langle A|\widehat{\mathrm{S}}_z|A\rangle\\
&= \frac{\hbar}{2}\begin{bmatrix}\cos(\omega t/2) & \sin(\omega t/2)\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\cos(\omega t/2)\\ \sin(\omega t/2)\end{bmatrix}\\
&= \frac{1}{2}\hbar\left(\cos^2(\tfrac{1}{2}\omega t) - \sin^2(\tfrac{1}{2}\omega t)\right)\\
&= \frac{1}{2}\hbar\cos(\omega t).
\end{aligned}$$

Answer F4

(a) We have

$$\left[\widehat{\mathrm{S}}_x, \widehat{\mathrm{H}}\right] = \omega\left[\widehat{\mathrm{S}}_x, \widehat{\mathrm{S}}_y\right] = \mathrm{i}\hbar\omega\,\widehat{\mathrm{S}}_z.$$

Using the generalized Ehrenfest theorem,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_x\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{S}}_x,\,\widehat{\mathrm{H}}\right]\right\rangle = \omega\langle S_z\rangle.$$

Also

$$\left[\widehat{\mathrm{S}}_y,\,\widehat{\mathrm{H}}\right] = \omega\left[\widehat{\mathrm{S}}_y,\,\widehat{\mathrm{S}}_y\right] = 0.$$

Using the generalized Ehrenfest theorem, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_y\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{S}}_y,\,\widehat{\mathrm{H}}\right]\right\rangle = 0.$$

Finally

$$\left[\widehat{\mathrm{S}}_z,\,\widehat{\mathrm{H}}\right] = \omega\left[\widehat{\mathrm{S}}_z,\,\widehat{\mathrm{S}}_y\right] = -\mathrm{i}\hbar\omega\widehat{\mathrm{S}}_x,$$

and using the generalized Ehrenfest theorem we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_z\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{S}}_z,\,\widehat{\mathrm{H}}\right]\right\rangle = -\omega\langle S_x\rangle.$$

(b) Using the results of part (a),

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle S_z\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}}{\mathrm{d}t}\langle S_z\rangle\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(-\omega\langle S_x\rangle\right)$$
$$= -\omega\frac{\mathrm{d}}{\mathrm{d}t}\langle S_x\rangle = -\omega^2\langle S_z\rangle.$$

(c) The general solution of the differential equation in part (b) is

$$\langle S_z\rangle = A\cos(\omega t) + B\sin(\omega t).$$

For the initial state $[1 \quad 0]^T$, the expectation value at time $t=0$ is $\langle S_z\rangle_0 = \frac{1}{2}\hbar$. Also the initial expectation value $\langle S_x\rangle_0 = 0$ and so at time $t = 0$ we have $[(\mathrm{d}/\mathrm{d}t)\langle S_z\rangle]_0 = 0$. Using these initial conditions gives

$$A = \frac{1}{2}\hbar, \quad B = 0.$$

Hence

$$\langle S_z\rangle = \frac{1}{2}\hbar\cos(\omega t),$$

which is consistent with the answer to Question F3.

Answer F5

(a)

$$\widehat{\mathrm{S}}_y\widehat{\mathrm{S}}_z - \widehat{\mathrm{S}}_z\widehat{\mathrm{S}}_y = \frac{1}{4}\hbar^2\left(\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} - \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\right)$$
$$= \frac{1}{4}\hbar^2\left(\begin{bmatrix}0 & \mathrm{i}\\ \mathrm{i} & 0\end{bmatrix} - \begin{bmatrix}0 & -\mathrm{i}\\ -\mathrm{i} & 0\end{bmatrix}\right)$$
$$= \frac{1}{2}\hbar^2\begin{bmatrix}0 & \mathrm{i}\\ \mathrm{i} & 0\end{bmatrix} = \frac{1}{2}\mathrm{i}\hbar^2\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = \mathrm{i}\hbar\,\widehat{\mathrm{S}}_x.$$

(b)

$$\langle S_x\rangle = \frac{1}{10}\hbar\,[1 \quad 2]\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}1\\ 2\end{bmatrix} = \frac{1}{10}\hbar\,[1 \quad 2]\begin{bmatrix}2\\ 1\end{bmatrix} = \frac{1}{10}\hbar\,(2+2) = \frac{2}{5}\hbar.$$

$$\langle S_y\rangle = \frac{1}{10}\hbar\,[1 \quad 2]\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix}\begin{bmatrix}1\\ 2\end{bmatrix} = \frac{1}{10}\hbar\,[1 \quad 2]\begin{bmatrix}-2\mathrm{i}\\ \mathrm{i}\end{bmatrix} = \frac{1}{10}\hbar\,(-2\mathrm{i}+2\mathrm{i}) = 0.$$

$$\langle S_z \rangle = \frac{1}{10}\hbar \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \frac{1}{10}\hbar \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ -2 \end{bmatrix} = \frac{1}{10}\hbar(1-4) = -\frac{3}{10}\hbar.$$

(c) Since the only possible result of a measurement of the square of a spin component is $\frac{1}{4}\hbar^2$,

$$\langle S_x^2 \rangle = \langle S_y^2 \rangle = \langle S_z^2 \rangle = \frac{1}{4}\hbar^2.$$

So

$$\Delta S_x = \left(\langle S_x^2 \rangle - \langle S_x \rangle^2\right)^{1/2} = \hbar \left(\frac{1}{4} - \frac{4}{25}\right)^{1/2} = \frac{3}{10}\hbar$$

$$\Delta S_y = \left(\langle S_y^2 \rangle - \langle S_y \rangle^2\right)^{1/2} = \hbar \left(\frac{1}{4} - 0\right)^{1/2} = \frac{1}{2}\hbar,$$

$$\Delta S_z = \left(\langle S_z^2 \rangle - \langle S_z \rangle^2\right)^{1/2} = \hbar \left(\frac{1}{4} - \frac{9}{100}\right)^{1/2} = \frac{2}{5}\hbar.$$

(d) Taking $A = S_x$, $B = S_y$, the generalized uncertainty relation is

$$\begin{aligned} \Delta S_x \, \Delta S_y &\geq \frac{1}{2} \left| \left\langle \left[\widehat{\mathrm{S}}_x, \widehat{\mathrm{S}}_y \right] \right\rangle \right| \\ &\geq \frac{1}{2} |\langle \mathrm{i}\hbar S_z \rangle| = \frac{1}{2}\hbar |\langle S_z \rangle|. \end{aligned}$$

This is satisfied as

$$\left(\frac{3}{10}\hbar\right) \left(\frac{1}{2}\hbar\right) \geq \left(\frac{1}{2}\hbar\right) \left(\frac{3}{10}\hbar\right),$$

i.e. the equality applies in this case.

Taking $A = S_y$, $B = S_z$, the generalized uncertainty relation is

$$\Delta S_y \, \Delta S_z \geq \frac{1}{2}\hbar |\langle S_x \rangle|.$$

This is satisfied as

$$\left(\frac{1}{2}\hbar\right) \left(\frac{2}{5}\hbar\right) \geq \left(\frac{1}{2}\hbar\right) \left(\frac{2}{5}\hbar\right),$$

with the equality applying once again.

Finally, taking $A = S_z$, $B = S_x$, the generalized uncertainty relation is

$$\Delta S_z \, \Delta S_x \geq \frac{1}{2}\hbar |\langle S_y \rangle|.$$

This is satisfied as

$$\left(\frac{2}{5}\hbar\right) \left(\frac{3}{10}\hbar\right) \geq \left(\frac{1}{2}\hbar\right) \times 0.$$

G: Dirac notation

Answer G1

Property	Dirac	Wave mechanics	Spin
Ket vector	$\lvert A\rangle$	$\Psi\,(x,t)$	$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$
Bra vector	$\langle A\rvert$	$\Psi^*(x,t)$	$[a_1^* \quad a_2^*]$
Inner product	$\langle A\vert B\rangle$	$\displaystyle\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Phi(x,t)\,\mathrm{d}x$	$[a_1^* \quad a_2^*]\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$
Normalization	$\langle A\vert A\rangle = 1$	$\displaystyle\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,\mathrm{d}x = 1$	$[a_1^* \quad a_2^*]\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = 1$
Expectation value	$\langle A\vert\widehat{\mathrm{O}}\vert A\rangle$	$\displaystyle\int_{-\infty}^{\infty} \Psi^*(x,t)\,\widehat{\mathrm{O}}\,\Psi(x,t)\,\mathrm{d}x$	$[a_1^* \quad a_2^*]\begin{bmatrix} \mathrm{O}_{11} & \mathrm{O}_{12} \\ \mathrm{O}_{21} & \mathrm{O}_{22} \end{bmatrix}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$

Answer G2

(a) **Generalized Ehrenfest theorem**

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{A}},\,\widehat{\mathrm{H}}\right]\right\rangle$$

In words, the rate of change of the expectation value of an observable A is equal to the expectation value of the commutator between $\widehat{\mathrm{A}}$ and the Hamiltonian $\widehat{\mathrm{H}}$ divided by $\mathrm{i}\hbar$.

Generalized uncertainty principle

$$\Delta A\,\Delta B \geq \frac{1}{2}\left|\left\langle\left[\widehat{\mathrm{A}},\,\widehat{\mathrm{B}}\right]\right\rangle\right|$$

In words, the product of the uncertainties of two observables A and B is greater than, or equal to, half the modulus of the expectation value of the commutator of $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{B}}$.

(b) Expanding the right-hand side we have

$$\begin{aligned}\widehat{\mathrm{B}}\left[\widehat{\mathrm{A}},\widehat{\mathrm{C}}\right] + \left[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\right]\widehat{\mathrm{C}} &= \widehat{\mathrm{B}}(\widehat{\mathrm{A}}\widehat{\mathrm{C}} - \widehat{\mathrm{C}}\widehat{\mathrm{A}}) + (\widehat{\mathrm{A}}\widehat{\mathrm{B}} - \widehat{\mathrm{B}}\widehat{\mathrm{A}})\widehat{\mathrm{C}} \\ &= \widehat{\mathrm{B}}\widehat{\mathrm{A}}\widehat{\mathrm{C}} - \widehat{\mathrm{B}}\widehat{\mathrm{C}}\widehat{\mathrm{A}} + \widehat{\mathrm{A}}\widehat{\mathrm{B}}\widehat{\mathrm{C}} - \widehat{\mathrm{B}}\widehat{\mathrm{A}}\widehat{\mathrm{C}} \\ &= \widehat{\mathrm{A}}\widehat{\mathrm{B}}\widehat{\mathrm{C}} - \widehat{\mathrm{B}}\widehat{\mathrm{C}}\widehat{\mathrm{A}} \\ &= \left[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\widehat{\mathrm{C}}\right].\end{aligned}$$

(c) We have the commutation relation

$$[\widehat{\mathrm{x}},\,\widehat{\mathrm{p}}_x] = \mathrm{i}\hbar$$

So the generalized uncertainty principle gives

$$\Delta x\,\Delta p_x \geq \frac{1}{2}\,\lvert\langle[\widehat{\mathrm{x}},\,\widehat{\mathrm{p}}_x]\rangle\rvert \geq \frac{1}{2}\,\lvert\langle\mathrm{i}\hbar\rangle\rvert = \frac{1}{2}\hbar.$$

For a free particle

$$\left[\widehat{\mathrm{x}},\,\widehat{\mathrm{H}}\right] = \frac{1}{2m}\left[\widehat{\mathrm{x}},\,\widehat{\mathrm{p}}_x^2\right] = \frac{1}{2m}\left[\widehat{\mathrm{x}},\,\widehat{\mathrm{p}}_x\,\widehat{\mathrm{p}}_x\right] = \frac{1}{2m}\left(\widehat{\mathrm{p}}_x\,[\widehat{\mathrm{x}},\,\widehat{\mathrm{p}}_x] + [\widehat{\mathrm{x}},\,\widehat{\mathrm{p}}_x]\,\widehat{\mathrm{p}}_x\right) = \frac{2\mathrm{i}\hbar}{2m}\,\widehat{\mathrm{p}}_x = \frac{\mathrm{i}\hbar}{m}\widehat{\mathrm{p}}_x.$$

So using the generalized Ehrenfest theorem,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{x}},\,\widehat{\mathrm{H}}\right]\right\rangle = \frac{\langle p_x\rangle}{m}.$$

(The classical analogue is the definition of linear momentum.)

Also,

$$\left[\widehat{\mathrm{p}}_x,\widehat{\mathrm{H}}\right] = \frac{1}{2m}\left[\widehat{\mathrm{p}}_x,\widehat{\mathrm{p}}_x^2\right] = 0.$$

So using the generalized Ehrenfest theorem,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{p}}_x,\, \widehat{\mathrm{H}}\right]\right\rangle = 0.$$

(The classical analogue is the conservation of linear momentum for a free particle.)

(d) As before

$$\Delta x\,\Delta p_x \geq \frac{1}{2}\hbar.$$

(This is a general result for any system.)

For a harmonic oscillator,

$$\begin{aligned}\left[\widehat{\mathrm{x}},\, \widehat{\mathrm{H}}\right] &= \left[\widehat{\mathrm{x}},\, \frac{1}{2m}\widehat{\mathrm{p}}_x^2 + \frac{1}{2}C\,\widehat{\mathrm{x}}^2\right] = \left[\widehat{\mathrm{x}},\, \frac{1}{2m}\widehat{\mathrm{p}}_x^2\right] + \left[\widehat{\mathrm{x}},\, \frac{1}{2}C\,\widehat{\mathrm{x}}^2\right]\\ &= \frac{\mathrm{i}\hbar}{m}\widehat{\mathrm{p}}_x + 0 = \frac{\mathrm{i}\hbar}{m}\widehat{\mathrm{p}}_x.\end{aligned}$$

So using the generalized Ehrenfest theorem,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{x}},\, \widehat{\mathrm{H}}\right]\right\rangle = \frac{1}{m}\langle p_x\rangle.$$

(This result is valid for any system with potential energy function $V(x)$.)

Also

$$\begin{aligned}\left[\widehat{\mathrm{p}}_x,\, \widehat{\mathrm{H}}\right] &= \left[\widehat{\mathrm{p}}_x,\, \frac{1}{2m}\widehat{\mathrm{p}}_x^2 + \frac{1}{2}C\,\widehat{\mathrm{x}}^2\right] = \left[\widehat{\mathrm{p}}_x,\, \frac{1}{2m}\widehat{\mathrm{p}}_x^2\right] + \left[\widehat{\mathrm{p}}_x,\, \frac{1}{2}C\,\widehat{\mathrm{x}}^2\right]\\ &= 0 + \frac{1}{2}C\,[\widehat{\mathrm{p}}_x,\, \widehat{\mathrm{x}}\widehat{\mathrm{x}}]\\ &= \frac{1}{2}C\,\left\{\widehat{\mathrm{x}}\,[\widehat{\mathrm{p}}_x,\, \widehat{\mathrm{x}}] + [\widehat{\mathrm{p}}_x,\, \widehat{\mathrm{x}}]\,\widehat{\mathrm{x}}\right\} = -\mathrm{i}\hbar\, C\,\widehat{\mathrm{x}}.\end{aligned}$$

So using the generalized Ehrenfest theorem,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{p}}_x,\, \widehat{\mathrm{H}}\right]\right\rangle = -C\,\langle x\rangle.$$

(This is the analogue of the classical equation of motion for a harmonic oscillator.)

Answer G3

(a) The operator $\widehat{\mathrm{H}}$ commutes with itself and so $\mathrm{d}\langle E\rangle/\mathrm{d}t = 0$. Hence $\langle E\rangle$ is a constant for any state.

(b) Similarly if $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{H}}$ commute, $\mathrm{d}\langle A\rangle/\mathrm{d}t = 0$ and so $\langle A\rangle$ is a constant for any state.

(c)

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\widehat{\mathrm{A}},\, \widehat{\mathrm{H}}\right]\right\rangle = \frac{1}{\mathrm{i}\hbar}\left\{\langle\widehat{\mathrm{A}}\widehat{\mathrm{H}}\rangle - \langle\widehat{\mathrm{H}}\widehat{\mathrm{A}}\rangle\right\}.$$

For a stationary state $|\Psi_n\rangle$, with $\widehat{\mathrm{H}}|\Psi_n\rangle = E_n|\Psi_n\rangle$,

$$\begin{aligned}\langle\widehat{\mathrm{A}}\widehat{\mathrm{H}}\rangle &= \langle\Psi_n|\widehat{\mathrm{A}}\widehat{\mathrm{H}}|\,\Psi_n\rangle = \langle\Psi_n|\widehat{\mathrm{A}}|\widehat{\mathrm{H}}\Psi_n\rangle\\ &= \langle\Psi_n|\widehat{\mathrm{A}}|E_n\Psi_n\rangle = E_n\langle\Psi_n|\widehat{\mathrm{A}}|\Psi_n\rangle,\end{aligned}$$

and

$$\begin{aligned}\langle\widehat{\mathrm{H}}\widehat{\mathrm{A}}\rangle &= \langle\Psi_n|\widehat{\mathrm{H}}\widehat{\mathrm{A}}|\Psi_n\rangle = \langle\Psi_n|\widehat{\mathrm{H}}\widehat{\mathrm{A}}\Psi_n\rangle\\ &= \langle\widehat{\mathrm{H}}\Psi_n|\widehat{\mathrm{A}}\Psi_n\rangle \quad \text{because } \widehat{\mathrm{H}} \text{ is Hermitian.}\\ &= \langle E_n\Psi_n|\widehat{\mathrm{A}}\Psi_n\rangle = E_n\langle\Psi_n|\widehat{\mathrm{A}}\Psi_n\rangle \quad \text{because } E_n \text{ is real.}\\ &= E_n\langle\Psi_n|\widehat{\mathrm{A}}|\Psi_n\rangle,\end{aligned}$$

where we have used the fact that $\widehat{\mathrm{H}}$ is Hermitian. So

$$\langle \widehat{\mathrm{A}}\widehat{\mathrm{H}} \rangle = \langle \widehat{\mathrm{H}}\widehat{\mathrm{A}} \rangle$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle = 0.$$

Hence $\langle A \rangle$ is a constant for a stationary state.

Answer G4

(a)

$$\langle A \rangle = \langle \Psi | \widehat{\mathrm{A}} | \Psi \rangle.$$

(b) Now

$$|\Psi\rangle = \sum_i a_i \, |\phi_i\rangle$$

and

$$\widehat{\mathrm{A}}|\phi_i\rangle = \lambda_i |\phi_i\rangle.$$

So

$$\widehat{\mathrm{A}}|\Psi\rangle = \sum_i a_i \, \widehat{\mathrm{A}}|\phi_i\rangle = \sum_i a_i \lambda_i |\phi_i\rangle$$

and

$$\langle \Psi | = \sum_j a_j^* \langle \phi_j |.$$

Hence

$$\langle A \rangle = \langle \Psi | \widehat{\mathrm{A}} | \Psi \rangle = \sum_i \sum_j a_j^* \, a_i \lambda_i \, \langle \phi_j | \phi_i \rangle = \sum_i \sum_j a_j^* \, a_i \, \lambda_i \, \delta_{ij}$$

$$= \sum_i a_i^* \, a_i \, \lambda_i = \sum_i |a_i|^2 \lambda_i,$$

as required.

(c) Now

$$|\Psi\rangle = \sum_i a_i |\phi_i\rangle$$

So

$$\langle \phi_n | \Psi \rangle = \sum_i a_i \langle \phi_n | \phi_i \rangle = \sum_i a_i \, \delta_{in} = a_n,$$

as required.

(d) The probability of a measurement $A = \lambda_n$ is

$$|\langle \phi_n | \Psi \rangle|^2 = |a_n|^2,$$

using the result of part (c).

(e) The probability of an outcome $A = \lambda_n$ is $|a_n|^2$ and so $\sum_i |a_i|^2 \lambda_i$ is the expectation value of the measurement of A. This is consistent with the answer to part (b).

Answer G5

(a) In Dirac notation, an operator $\widehat{\mathrm{A}}$ is Hermitian if

$$\langle \psi_1 | \widehat{\mathrm{A}} \psi_2 \rangle = \langle \widehat{\mathrm{A}} \psi_1 | \psi_2 \rangle \quad \text{for normalizable } \psi_1 \text{ and } \psi_2.$$

In one-dimensional wave mechanics, this condition is

$$\int_{-\infty}^{\infty} \psi_1^*(x) \left[\widehat{\mathrm{A}}\, \psi_2(x)\right] \mathrm{d}x = \int_{-\infty}^{\infty} \left[\widehat{\mathrm{A}} \psi_1(x)\right]^* \psi_2(x) \, \mathrm{d}x.$$

In spinor notation, the corresponding matrix A is Hermitian if $A_{ij} = A_{ji}^*$, i.e. if

$$A^* = A^T.$$

(b) Using integration by parts,

$$\begin{aligned}
\int_{-\infty}^{\infty} \psi_1^* \left(\widehat{\mathrm{p}}_x \, \psi_2\right) \mathrm{d}x &= \int_{-\infty}^{\infty} \psi_1^* \left(-\mathrm{i}\hbar \frac{\partial}{\partial x} \psi_2\right) \mathrm{d}x \\
&= -\mathrm{i}\hbar \left(\left[\psi_1^* \, \psi_2\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \psi_1^*}{\partial x} \psi_2 \, \mathrm{d}x \right) \\
&= \int_{-\infty}^{\infty} \left(-\mathrm{i}\hbar \frac{\partial}{\partial x} \psi_1\right)^* \psi_2 \, \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\widehat{\mathrm{p}}_x \, \psi_1\right)^* \psi_2 \, \mathrm{d}x,
\end{aligned}$$

where we have used the fact that ψ_1 and ψ_2 tend to zero as x tends to $\pm\infty$. So $\widehat{\mathrm{p}}_x = -\mathrm{i}\hbar\partial/\partial x$ is a Hermitian operator.

(c)

$$\begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}^* = \begin{bmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{bmatrix} = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}^T.$$

So $\widehat{\mathrm{S}}_y$ is Hermitian.

Answer G6

(a) If ϕ_i and ϕ_j are eigenfunctions of a Hermitian operator $\widehat{\mathrm{A}}$ with corresponding eigenvalues λ_i and λ_j, the Hermitian condition for $\widehat{\mathrm{A}}$ gives

$$\langle \phi_j | \widehat{\mathrm{A}} \phi_i \rangle = \langle \widehat{\mathrm{A}} \phi_j | \phi_i \rangle.$$

So

$$\langle \phi_j | \lambda_i \, \phi_i \rangle = \langle \lambda_j \, \phi_j | \phi_i \rangle,$$

that is

$$\lambda_i \langle \phi_j | \phi_i \rangle = \lambda_j^* \langle \phi_j | \phi_i \rangle,$$

thus

$$\left(\lambda_i - \lambda_j^*\right) \langle \phi_j | \phi_i \rangle = 0. \qquad (*)$$

Putting $i = j$, we obtain

$$\left(\lambda_i - \lambda_i^*\right) \langle \phi_i | \phi_i \rangle = 0.$$

But the inner product of any (non-zero) vector with itself is non-zero, and so

$$\lambda_i - \lambda_i^* = 0.$$

Hence the eigenvalue λ_i is real.

(b) Using the result in Equation (*) we obtain

$$\left(\lambda_i - \lambda_j\right) \langle \phi_j | \phi_i \rangle = 0.$$

If $\lambda_i \neq \lambda_j$, this gives

$$\langle \phi_j | \phi_i \rangle = 0,$$

Hence ϕ_i and ϕ_j are orthogonal.

(c) The expectation value of an observable A is

$$\langle A\rangle = \langle\Psi|\widehat{\mathrm{A}}\Psi\rangle$$

So

$$\langle A\rangle^* = \langle\Psi|\widehat{\mathrm{A}}\Psi\rangle^* = \langle\widehat{\mathrm{A}}\Psi|\Psi\rangle.$$

Because $\widehat{\mathrm{A}}$ is Hermitian, this gives

$$\langle A\rangle^* = \langle\Psi|\widehat{\mathrm{A}}\Psi\rangle = \langle A\rangle.$$

The condition $z^* = z$ guarantees that z is real, so the expectation value of a Hermitian operator is real.

H: Three-dimensional systems

Answer H1

(a) The normalization condition is

$$1 = \int_0^\infty \int_0^{2\pi} |\psi|^2 r\,\mathrm{d}\phi\,\mathrm{d}r = \int_0^\infty \int_0^{2\pi} A^2 r^3 \exp\left(-r^2/a^2\right)\,\mathrm{d}\phi\,\mathrm{d}r$$

$$= 2\pi A^2 \int_0^\infty r^3 \exp\left(-r^2/a^2\right)\,\mathrm{d}r$$

$$= 2\pi A^2 a^4 \int_0^\infty u^3 \exp\left(-u^2\right)\,\mathrm{d}u,$$

where we have used the substitution $u = r/a$. The remaining integral is given in the question, so

$$1 = (2\pi\, a^4\, A^2)\left(\frac{1}{2}\right) = \pi a^4\, A^2.$$

Hence the real positive normalization constant is

$$A = \frac{1}{\sqrt{\pi}a^2}.$$

(b)

$$\widehat{\mathrm{L}}_z\psi = -\mathrm{i}\hbar\frac{\partial\psi}{\partial\phi} = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}\left(A\mathrm{e}^{-\mathrm{i}\phi}\, r\,\exp(-r^2/2a^2)\right)$$

$$= -\mathrm{i}\hbar(-\mathrm{i})\psi$$

$$= -\hbar\psi.$$

So ψ is an eigenfunction of $\widehat{\mathrm{L}}_z$ with eigenvalue $-\hbar$. So the expectation values are

$$\langle L_z\rangle = -\hbar, \quad \langle L_z^2\rangle = \hbar^2$$

and the uncertainty is $\Delta L_z = 0$. Note that we could also have found the expectation values by using the sandwich rule.

(c) The measurement will definitely return the value $-\hbar$.

Answer H2

(a) The expectation value of r is given by the integral

$$\langle r\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} r|\psi|^2 r^2 \sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta\,\mathrm{d}r$$

$$= \left(\frac{1}{a\sqrt{\pi}}\right)^3 \int_0^\infty \int_0^\pi \int_0^{2\pi} r^3 \exp\left(-\frac{r^2}{a^2}\right)\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta\,\mathrm{d}r$$

$$= 4\pi\left(\frac{1}{a\sqrt{\pi}}\right)^3 \int_0^\infty r^3 \exp\left(-r^2/a^2\right)\,\mathrm{d}r.$$

We make the substitution $u = r/a$. Then $r = au$, $\mathrm{d}r = a\,\mathrm{d}u$ and the limits of integration become $u = 0$ and $u = \infty$. Hence

$$\langle r\rangle = \left(\frac{4a}{\sqrt{\pi}}\right)\int_0^\infty u^3 \exp\left(-u^2\right)\,\mathrm{d}u = \frac{2a}{\sqrt{\pi}},$$

where we have used the first standard integral given in the question.

(b) Similarly,

$$\begin{aligned}\langle r^2\rangle &= 4\pi\left(\frac{1}{a\pi^{1/2}}\right)^3\int_0^\infty r^4 \exp\left(-r^2/a^2\right)\,\mathrm{d}r\\ &= \frac{4a^2}{\sqrt{\pi}}\int_0^\infty u^4 \exp\left(-u^2\right)\,\mathrm{d}u\\ &= 3a^2/2.\end{aligned}$$

Therefore

$$\begin{aligned}(\Delta r)^2 &= \langle r^2\rangle - \langle r\rangle^2\\ &= a^2\left(\frac{3}{2} - \frac{4}{\pi}\right)\\ &= 0.227\,a^2.\end{aligned}$$

Hence the uncertainty is $\Delta r = 0.476\,a$.

Answer H3

(a) The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) = E\psi,$$

for $0 \le x \le L,\ 0 \le y \le L,\ 0 \le z \le L.$

The boundary conditions are

$$\begin{aligned}&\psi(0, y, z) = 0, \quad \psi(L, y, z) = 0,\\ &\psi(x, 0, z) = 0, \quad \psi(x, L, z) = 0,\\ &\psi(x, y, 0) = 0, \quad \psi(x, y, L) = 0.\end{aligned}$$

(b) Now

$$\begin{aligned}\frac{\partial^2\psi}{\partial x^2} &= \frac{\partial^2}{\partial x^2}(A\sin(k_x x)\sin(k_y y)\sin(k_z z))\\ &= -Ak_x^2\sin(k_x x)\sin(k_y y)\sin(k_z z)\\ &= -k_x^2\psi.\end{aligned}$$

There are similar equations for the y and z derivatives. Hence, substituting in the differential equation gives

$$\frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = E.$$

The boundary condition $\psi(0, y, z) = 0$ is automatically satisfied. The boundary condition $\psi(L,\ y,\ z) = 0$ leads to $k_x L = n_x\pi$, i.e. $k_x = n_x\pi/L$. Similarly, $k_y = n_y\pi/L$ and $k_z = n_z\pi/L$. So

$$E = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2),$$

where n_x, n_y and n_z are integers. If any of these integers is zero, then $\psi(x, y, z) = 0$ everywhere, which is not an interesting solution. If any of the integers is negative, we get the same solution as for positive integers, possibly multiplied by a phase factor. We can therefore restrict n_x, n_y and n_z to be *positive* integers $1, 2, 3\ldots.$

(c) (i) Using $\sin B \cos C = \frac{1}{2}(\sin(B+C) + \sin(B-C))$,

$$\Psi(x,y,z,0) = \frac{A}{2}\sin(\pi x/L)\sin(2\pi y/L)\left\{\sin(6\pi z/L) - \sin(2\pi z/L)\right\},$$

which is a linear superposition of two energy eigenfunctions with $n_x = 1$, $n_y = 2$, $n_z = 6$ and $n_x = 1$, $n_y = 2$, $n_z = 2$. The corresponding energies are $41\pi^2\hbar^2/2mL^2$ and $9\pi^2\hbar^2/2mL^2$. These are the possible outcomes of a measurement of energy, each with probability 0.5.

(ii)

$$\Psi(x,y,z,t) = \frac{2}{L^{3/2}}\sin(\pi x/L)\sin(2\pi y/L)\{\sin(6\pi z/L)\exp(-\mathrm{i}41\pi^2\hbar t/2mL^2) - \sin(2\pi z/L)\exp(-\mathrm{i}9\pi^2\hbar t/2mL^2)\}.$$

Answer H4

(a) The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) - \frac{e^2}{4\pi\varepsilon_0 r}\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

(b)

$$-\frac{\hbar^2}{2mr}\frac{\mathrm{d}^2}{\mathrm{d}r^2}(r\psi(r)) - \frac{e^2}{4\pi\varepsilon_0 r}\psi(r) = E\psi(r).$$

(c) If $\psi(r) = A\exp(-\lambda r)$ then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}r}(r\psi) &= A\frac{\mathrm{d}}{\mathrm{d}r}(r\exp(-\lambda r))\\ &= A(1-\lambda r)\exp(-\lambda r)\end{aligned}$$

and

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}r^2}(r\psi) &= A\left\{-\lambda\exp(-\lambda r) - \lambda(1-\lambda r)\exp(-\lambda r)\right\}\\ &= A\left(-2\lambda + \lambda^2 r\right)\exp(-\lambda r).\end{aligned}$$

Substituting in the time-independent Schrödinger equation, we obtain

$$-\frac{\hbar^2}{2mr}A(-2\lambda + \lambda^2 r)\exp(-\lambda r) - \frac{e^2}{4\pi\varepsilon_0 r}A\exp(-\lambda r) = EA\exp(-\lambda r).$$

Equating terms in $1/r$ gives

$$\frac{\hbar^2\lambda}{m} - \frac{e^2}{4\pi\varepsilon_0} = 0,$$

which leads to

$$\lambda = \frac{me^2}{4\pi\varepsilon_0\hbar^2},$$

as required.

Equating constant terms gives

$$E = -\frac{\hbar^2\lambda^2}{2m} = -\frac{1}{(4\pi\epsilon_0)^2}\frac{me^4}{2\hbar^2}.$$

(d) The normalization condition is $4\pi\int_0^\infty |\psi(r)|^2 r^2\,\mathrm{d}r = 1$. So, using the substitution $2\lambda r = u$,

$$\begin{aligned}1 &= 4\pi|A|^2\int_0^\infty \exp(-2\lambda r)r^2\,\mathrm{d}r\\ &= 4\pi|A|^2\frac{1}{(2\lambda)^3}\int_0^\infty \exp(-u)u^2\,\mathrm{d}u\\ &= \frac{\pi|A|^2}{\lambda^3}.\end{aligned}$$

Choosing A to be real and positive, the normalization constant is

$$A = \left(\frac{\lambda^3}{\pi}\right)^{1/2} = \frac{1}{\sqrt{\pi}}\left(\frac{me^2}{4\pi\epsilon_0\hbar^2}\right)^{3/2}.$$